International Conference on
EXTENDED DEFECTS IN SEMICONDUCTORS
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Organized by:

**Institute of Physics of the Polish Academy of Sciences,
Warszawa, Poland
Georg-August-Universität, Göttingen, Germany
Institut für Halbleiterphysik, Frankfurt (Oder), Germany**

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PROGRAMME AND ABSTRACTS

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CONFERENCE PROGRAMME

Sunday, September 6

Arrival of participants, registration

From 18:00 **dinner and welcoming glass of wine**

Monday, September 7

8:00 **breakfast**

Morning session:

9:05 - 9:20 Opening address

9:20 - 10:00 H. P. Strunk, Erlangen, Germany
Relaxation of misfit-induced strain in semiconductor heterostructures

10:00 - 10:40 E. A. Fitzgerald, Cambridge, USA
Dislocations in relaxed SiGe/Si heterostructures

10:40 - 11:10 **coffee break**

11:10 - 11:50 V. I. Vdovin, Moscow, Russia
Misfit dislocations in epitaxial heterostructures: mechanisms of generation and multiplication

11:50 - 12:30 B. Pichaud, Marseille, France
Dislocation mechanisms involved in the relaxation of heteroepitaxial semiconducting systems

12:30 - 12:50 J. Kątcki, Warsaw, Poland
Formation of dislocations in InGaAs/GaAs heterostructures

13:00 **lunch**

Afternoon session:

17:00 - 17:40 T. Wosiński, Warsaw, Poland
Quantum interference at misfit dislocations in III-V heterostructures

17:40 - 18:20 V. V. Kveder, Chernogolovka, Russia
Electronic properties of regular dislocations in silicon

18:20 - 18:40 S. Mil'shtein, Lowell, USA
Crystalline defects as enhancement and limits to microminiaturization

Evening:

19:00 **Get together at the bonfire**

Tuesday, September 8

8:00 **breakfast**

Morning session:

9:00 - 9:40 R. Hull, Charlottesville, USA
Interactions of moving dislocations in semiconductors with point, line and planar defects

9:40 - 10:20 K. Sumino, Sendai, Japan
Impurity reaction with dislocations in semiconductors

10:20 - 10:50 **coffee break**

10:50 - 11:30 S. Pizzini, Milan, Italy
Chemistry and physics of segregation of impurities at extended defects in silicon

11:30 - 12:10 M. Seibt, Göttingen, Germany
Structural and electrical properties of metal silicide precipitates in silicon

12:10 - 12:30 P. Alippi, Milan, Italy
From point to extended self-interstitials in silicon: a tight-binding molecular dynamics study

12:30 **lunch**

Afternoon: Mountains hiking

18:00 **dinner**

Evening session:

19:00 - 19:40 A. George, Nancy, France
Dislocation nucleation and multiplication at crack tips in silicon

19:40 - 20:20 L. I. Fedina, Novosibirsk, Russia
Extended defects formation in Si crystals at clustering of intrinsic point defects studied by High Resolution Electron Microscopy

20:30 - 22:00 POSTER SESSION

Wednesday, September 9

8:00 **breakfast**

Morning session:

9:00 - 9:40 H. Alexander, Cologne, Germany
Kinks on partials of 60°-dislocations in silicon as revealed by a new TEM-technique

9:40 - 10:20 Yu. L. Iunin & V. I. Nikitenko, Chernogolovka, Russia
Dislocation kink dynamics in crystals with deep Peierls potential relief

10:20 - 10:50 **coffee break**

10:50 - 11:30 Y. Yamashita, Okayama, Japan
Hydrogen enhanced dislocation glides in silicon

11:30 - 12:10 V. V. Bulatov, Cambridge, USA
Dislocation mobility in Si: from atomic core to micron scale

12:10 - 12:30 I. Yonenaga, Sendai, Japan
Recombination-enhanced dislocation motion in SiGe and Ge

12:30 **lunch**

Afternoon:

13:30 - 19:00 **Sightseeing tour**

Evening:

20:00 **Conference dinner**

Thursday, September 10

8:30 **breakfast**

Morning session:

9:30 - 10:10 T. Suski, Warsaw, Poland
Growth and properties of bulk single crystals of GaN; role of defects

10:10 - 10:50 Z. Liliental-Weber, Berkeley, USA
Extended defects in GaN

10:50 - 11:20 **coffee break**

11:20 - 12:00 J.-L. Rouviere, Grenoble, France
Structural characterization of extended defects in GaN epilayers and AlN/GaN heterostructures by Transmission Electron Microscopy

12:00 - 12:40 G. Salviati, Parma, Italy
CL and TEM study of optically active defects in GaN and AlGaN epilayers grown on sapphire

13:00 **lunch**

Afternoon session:

17:00 - 17:40 R. Jones, Exeter, UK
The interaction of oxygen with dislocations in GaN

17:40 - 18:00 P. Pirouz, Cleveland, USA
Deformation of single crystal 4H- and 6H-SiC

18:00 **dinner**

Evening session:

19:00 - 20:30 PANEL DISCUSSION, animated by E. R. Weber, Berkeley, USA
on: *The role of dislocations and other extended defects in GaN*

20:30 - 22:00 POSTER SESSION

Friday, September 11

8:00 **breakfast**

Morning session:

9:00 - 9:40 H.-J. Möller, Freiberg, Germany
Oxygen and carbon precipitation in multicrystalline solar silicon

9:40 - 10:20 T. V. Torchinskaya, Kiev, Ukraine
Recombination-enhanced microprecipitate formation in LPE GaAs structures

10:20 - 10:50 **coffee break**

10:50 - 11:10 H. S. Leipner, Halle, Germany
Positron annihilation at dislocations and related point defects in semiconductors

11:10 - 11:30 E. A. Steinman, Chernogolovka, Russia
The relation between misfit dislocation structure and PL in $Si_{1-x}Ge_x$ /Si (100) heterostructures

11:30 - 11:50 Closing of EDS'98

12:30 **lunch**

Note that all the posters will be on display during the whole conference, although two official POSTER SESSIONS are scheduled in the Programme.

ABSTRACTS

The number placed after the letter P at the upper right corner of an abstract denotes the number of the poster board.

Relaxation of Misfit-induced Strain in Semiconductor Heterostructures

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The properties of mismatched heteroepitaxial systems during growth and subsequent processing is influenced by the built-in misfit strain. The systems generally tend to relax this strain and the direction of the processes are thermodynamically described towards reduction in the total Gibbs free energy. Usually the mechanisms are grouped into plastic and elastic relaxation mechanisms and we will in addition consider diffusive mechanisms. We also will outline their mutual dependencies and exemplify the discussion with results obtained from the system SiGe on Si. Plastic mechanisms involve misfit dislocations and numerous details of dislocation nucleation, glide, climb and multiplication have been elaborated in the past decades. The diffusive mechanisms consist essentially in a readjustment in the concentration profiles at and near the interfaces. The elastic mechanisms became important when strained superlattices had to be grown. These mechanisms consist essentially in an efficient inhomogeneous redistribution of misfit strain by a modulation of the initially planar growth surface. Two modulation types, rippling and islanding, are prominent and are generally considered typical of low and high misfit systems, resp. Our results, however, indicate that they are closely related. We will show that infact islands are the ultimate state. Moreover frequently pores or grooves are the real relaxational structure element.

When the epitaxial layers exhibit a rather low crystal symmetry, interesting modifications of the relaxation phenomena can be observed. We will discuss examples taken from wurtzite III-nitride growth. We consider short range strain compensation via differently orientated 'grainlets' with opposite sign of the misfit. This mechanism implies a tendency to polycrystallinity although epitaxial growth is involved. As a most recent result we will dwell on planar inclusions with cubic crystal structure in an otherwise single crystalline wurtzite GaInN. These inclusions are, due to a slightly smaller lattice parameter, sources of elastic strain. This strain, however, does not compensate the misfit strain (rather it enhances it in our example), but -via the piezoelectric effect- it counteracts high electric fields that would form otherwise in the wurtzite phase due to spontaneous polarization.

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Dislocations in Relaxed SiGe/Si Heterostructures

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Relaxed SiGe layers on Si offer a means to integrate SiGe FETs, Si-based MEMs, and III-V electronics and optoelectronics on Si substrates. However, these applications require that the SiGe layers are substantially relaxed, thereby necessitating the introduction of a high density of dislocations. We have extensively explored SiGe layers with graded compositions for obtaining great relaxation with a minimal number of threading dislocations penetrating the top surface. We have explained the need for the residual dislocation density with a kinetic model of dislocation flow during a constant strain rate created by the graded growth. Subsequently, we have discovered that an increase in threading dislocation density at the surface with increased deformation by grading to greater Ge concentrations is connected to the deleterious interaction of the surface morphology with the strain fields of underlying dislocations. This interaction leads to the formation of dislocation pile-ups in the graded structure, and due to the immobility of the threading dislocations, more dislocations need to be nucleated, increasing the threading dislocation density and rendering high-concentration Ge alloys useless for minority carrier devices.

However, recognizing that the surface morphology is a key factor in the pile-up formation, we have applied a planarization step within the graded buffer to free the pinned dislocations upon subsequent continued graded layer growth. This process has a drastic effect on the residual threading dislocation density and on the number of dislocation pile-ups. Essentially, the planarization does indeed free the pinned threading dislocations, allowing them to glide and relieve strain. In addition, the threading dislocation density actually decreases with subsequent grading, creating a Ge on Si structure with a lower defect density than the dislocation density observed at 50% Ge, the point at which planarization occurred. This remarkable reduction has revealed new insight into dislocation processes in relaxed heterostructures and has allowed us to consider new structures for further threading dislocation reduction.

Finally, the integration of Ge and III-V materials with Si using these SiGe layered structures creates a thermal-mismatch problem for large-area devices such as solar cells. If the structures are relaxed at the growth temperature, then upon cooling, a tensile stress is induced into the Ge and/or GaAs layers. For thick structures, this stress may be great enough to crack the epitaxial layers. We show that by using SiGe interlayers, it is possible to introduce compressive strain into the buffer structure, compensating for the tensile strain that accumulates upon cooling from the growth temperatures. Dislocation interaction in the graded layer help retain some of the compressive strain, allowing the structure to remain slightly compressive even at room temperature, aiding subsequent integration of GaAs layers without cracking. We have fabricated near-ideal Ge photodiodes from this Ge on Si, and we have also grown GaAs on this Ge with unprecedented crystal quality.

MISFIT DISLOCATIONS IN EPITAXIAL HETEROSTRUCTURES: MECHANISMS OF GENERATION AND MULTIPLICATION

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Relaxation of misfit strains in heterostructures occurs through formation of misfit dislocations at the interface during epitaxial growth or subsequent annealing. The extent to which lattice mismatch is accomodated by misfit dislocations depends on the efficiency of dislocation processes of nucleation, propagation and multiplication. The contribution of each of these processes to the formation of the final dislocation structure depends on a number of factors: lattice mismatch, growth temperature, layer thickness, substrate orientation and others. For heterostructures with equal or similar growth conditions, remarkable differences observed in dislocation structure are determined by the nature of materials contacting at the interface and, in particular, by alloy composition. The knowledge of dislocations behavior patterns in each heterosystem allows to control the dislocation structure of materials. For example, recently the idea of growing epitaxial layers with low threading dislocation density due to the effect of substrate plastic deformation has been successfully realized in GeSi/Si and GaInAs/GaAs heterosystems.

In this work, the regularities of dislocation structure formation in single layer heterostructures with low lattice mismatch ($f<1\%$) are reviewed. The emphasis is on the recently suggested mechanisms of dislocation nucleation and multiplication. The correspondence of the suggested models to real processes occurring in materials is evaluated. The misfit dislocation network was found to transform in some heterostructures from regular flat to dense three-dimensional during the epitaxial growth. Such evolution of the misfit dislocation network results from the operation of several dislocation generation and multiplication mechanisms. Experimentally observed features of dislocation structure formation are treated in terms of the influence of the nature of materials contacting at the interface on the dislocations behavior. Special emphasis is made on the role of microsegregations and intrinsic point defects in the alloy matrix in dislocation generation, propagation and multiplication. The discussed questions are illustrated by experimental results obtained on the heterostructures based on SiGe and III-V quaternary alloys.

DISLOCATION MECHANISMS INVOLVED IN THE RELAXATION OF HETEROEPITAXIAL SEMICONDUCTING SYSTEMS.

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Growing a thin coherent epitaxial layer on a substrate of the same structure but a different lattice parameter, yields to a strained layer which can store an enormous elastic energy since this last is proportional to the square of the misfit (relative difference between the film and substrate lattice parameters). So increasing the film thickness it will become energetically more favourable to relax this energy. Several relaxation routes exist: rippling of the layer surface, islanding interdiffusion etc..., but in this review paper we will rather focus on dislocation induced relaxation mechanisms which are very frequent at usual crystal growth and processing temperatures for an epilayer/substrate system with a misfit below 3%.

The different steps of the plastic relaxation of the system, which take place as soon as a critical thickness is reached, are very similar to those involved in bulk plasticity of semiconductors: nucleation, development, interactions and multiplication of dislocations, but they exhibit some original features due to the confinement of high strains in the film and/or at the interface.

The nucleation of dislocations is a difficult process specially in low misfit systems which favours layer metastability. Although the mechanism proposed by Matthews[1] has been observed it is not able to produce misfit dislocations in sufficiently high density to relax the film stress. Heterogeneous nucleation events can help this relaxation but they are closely related to the experimental peculiarities so that no intrinsic critical thickness can be defined.

The dislocation development across large distances is needed to produce misfit dislocation lengths compatible with the sample size, so the dislocation mobility at the different steps of the growing process (growth period, cooling) is a controlling parameter of the relaxation. Metastability can be expected for experimental conditions in which the dislocation mobility is low.

The interaction of dislocations is favoured in epitaxial systems as compared with bulk samples because of the occurence of multiple glide systems and of the existence of the interface at which or in the vicinity of which dislocations are forced to meet. These interactions impede[2] or inhibit the dislocation motion retarding or freezing the relaxation.

From interactions, multiplication events [3] can be initiated allowing misfit dislocations to be produced further. These relaxation helping processes are, as in the bulk, based on the cross slip of dislocations a mechanism which allows to overcome the blocking interaction. Nevertheless, increasing the dislocation density in the film yields to a hardening phenomenon and to imcomplete relaxation of the system.

These different steps of the relaxation will be discussed, some models will be presented and compared with experimental results in different epitaxial systems, GaAs/Ge, SiGe/Si, GaInAs/GaAs, Si/Si(n+) etc...

[1] Matthews J.W. and Blakeslee A.E., J. Cryst. Growth **27** (1974) 118; **29** (1975) 273; **32** (1976) 265
[2] Freund L.B., J. Appl. Phys. **68** (1990) 2073
[3] Lefebvre A., Herbeaux C and Di Persio J., Phil.Mag. A **63** (1991) 471

QUANTUM INTERFERENCE AT MISFIT DISLOCATIONS IN III-V HETEROSTRUCTURES

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In this lecture we discuss a phenomenon of quantum interference of charge carriers flowing around misfit dislocations in heterostructures of III-V compound semiconductors. Misfit dislocations are formed at the interface in these heterostructures during their epitaxial growth to accommodate lattice mismatch between the substrate and the epilayer. Localized states of the dislocation core usually accept majority carriers from the corresponding energy band, thus causing that the dislocation line becomes electrically charged and is screened by a cylindrical region (so-called Read's cylinder) of the space charge of opposite sign, formed by ionized donors or acceptors.

We have found that misfit dislocations, generated in GaAsSb/GaAs heterostructures with a small lattice mismatch, give rise to low-temperature magnetoconductance oscillations periodic in magnetic field. We interpret these oscillations in terms of the Aharonov-Bohm interference of charge carriers flowing across an array of parallel dislocations. Under strong magnetic field, applied parallel to the dislocation axes, localised orbits encircling Read's cylinders around dislocations are formed cyclically whenever the magnetic flux enclosed inside the cylinder is changed by one flux unit *h/e*. Capture of free charge carriers on these quasi-stationary orbits give rise to oscillations of the structure conductance. We propose a semi-quantitative model which explains all the characteristic features of the observed phenomenon.

This work has been supported by the Committee for Scientific Research of Poland under Grant No 2 P03B 028 13.

THE ELECTRONIC PROPERTIES OF REGULAR DISLOCATIONS IN SILICON

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The main topic of a talk is a discussion of a present day picture of electronic properties of clean dislocations in silicon and possible influence of impurities contamination on these properties. The results obtained using the photoluminescence (PL), electric-dipole spin resonance, ODMR, EBIC and DLTS show that the main activity of regular straight segments of clean dislocations is attributed to one-dimensional energy bands caused by the deformation potential of dislocations. The localization length L of electrons and holes in these bands and their mobility are rather high. In case of straight dislocations L is more than 1000A and the mobility decreases when temperature increases. The overheating of one-dimensional electrons by microwave electric field and some other non-linear effects were observed in this case. A model explaining the temperature dependence of the dislocation-related luminescence is suggested. Using this model it is possible to optimize the dislocation structure to increase the PL intensity. In particular, the p-n junctions made on properly prepared samples exhibit the dislocation-related electro-luminescence at 0.8eV even at room temperature. It is shown that the energy bands caused by a deformation potential also play an important role in recombination of carriers on deep dislocation-related states, caused by impurities and other defects existing in the vicinity of dislocation.

INTERACTIONS OF MOVING DISLOCATIONS IN SEMICONDUCTORS WITH POINT, LINE AND PLANAR DEFECTS

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The synthesis of thin strained epitaxial semiconductor layers provides broad new avenues for the study of dislocation energetics and kinetics. In particular, such heterostructures enable the effective stress on misfit dislocations, and the length of the propagating dislocation segment to be accurately tuned and quantified over stress ranges 100 MPa - 1 GPa, and length scales 10 - 1000 nm. In addition, fundamental interactions between propagating dislocations and a range of crystalline defects may be quantitatively probed.

In this paper, we use design of strained layer (Si)/Ge_xSi_{1-x}/Si heterostructures to explore dislocation - defect interactions. Point defects are controllably introduced using ion implantation into the heterostructure surface. The density and spatial distribution of these defects can be controlled via the implant dose, species and energy. The interactions of dislocations with these point defects are then studied via the dislocation propagation kinetics as functions of the implant distribution. It is found that significant modification of dislocation velocities occur as a function of the implant conditions. Systematic analysis of these effects as functions of ion dose and current and epilayer stress provides mechanistic understanding of the operative dislocation - point defect interactions. Inter-dislocation interactions are also studied by observing the passage of propagating dislocations past pre-existing interfacial misfit dislocations. These observations are performed real-time during growth of Ge_xSi_{1-x}/Si heterostructures in a unique ultra-high vacuum transmission electron microscope (UHV-TEM) equipped with an in-situ Ge_xSi_{1-x}/Si CVD (Chemical Vapor Deposition) growth system [1]. Finally dislocation - surface interactions are probed using the same UHV-TEM-CVD system by studying dislocation motion as a function of the surface chemistry. It is observed, for example, that large enhancements of misfit dislocation motion through a Ge_xSi_{1-x}/Si heterostructure are observed with the presence of a surface oxide, in comparison to an atomically clean surface.

In summary these experiments enable us to quantify the effects of dislocation - defect interactions in strained layer heterostructures. These observations are currently being incorporated into a "process simulator" we have developed for prediction of misfit dislocation densities and properties during growth and electronic device processing of strained layer heterostructures. The predictive capabilities of this process simulator will be demonstrated.

[1] *Work performed in conjunction with R. Tromp, F. Ross and M. Reuter at IBM Yorktown Heights Research Center.*

IMPURITY REACTION WITH DISLOCATIONS IN SEMICONDUCTORS

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Reaction between dislocations and impurities in semiconductors is not only interesting scientifically but is also very important technologically. It results in the change in the kinetic properties of dislocations, leading to the hardening of the crystal, and also the changes in the electrical and optical properties of dislocations. Simultaneously, it brings about the spatial variation in the impurity distribution within the crystal. This paper discusses some important aspects concerning dislocation-impurity reactions on the basis of the work of author's group.

Impurity Segregation/Precipitation/Gettering at Dislocations

Development of impurity atmosphere and precipitation at a dislocation are often confused in literature. Impurities remain as impurities in the former while particles of a new phase are formed in the latter. The driving force for segregation is the interaction between a dislocation and an individual impurity atom mainly through their strain fields. On the other hand, the driving force for preferential precipitation at a dislocation is the liberation of the energies associated with impurity supersaturation and highly disturbed atomic arrangement at the dislocation core. The atomic structure of a precipitate developed at the dislocation core is not necessarily the same as that developed in the matrix region. A thermodynamical calculation shows that impurity atmosphere is never developed around a dislocation for typical impurity concentrations in semiconductors, for example 10 ppm or less. Thus, practically, impurity gettering at a dislocation takes place by means of preferential precipitation of supersaturated impurities.

Role of Precipitate Morphology on Dislocations

Preferential precipitation of supersaturated oxygen impurities on dislocations makes a Si crystal hard. The morphology of oxygen precipitates on a dislocation depends on the temperature and duration of annealing in a quite different way from that in the Si matrix. In the early stage of precipitation precipitates are developed as thin cylinders along the dislocation line and replace the dislocation core. In the intermediate stage precipitates on a dislocation become discretely distributed along the dislocation line. Both the size and separation of the precipitates increase as precipitation proceeds. Correspondingly, the maximum pinning of a dislocation and, as a result, the highest strength of the Si crystal is achieved at an intermediate stage of oxygen precipitation on the dislocation. Such variation of precipitate morphology on a dislocation with precipitation process can well be interpreted with an energy consideration.

Gettering of Metallic Impurities at Dislocations

Precipitation of metallic impurities at a dislocation in Si shows a quite rich variety of behaviour, depending on many parameters such as the species and concentration of impurities, the type of dislocation, and the cooling rate of crystal. Fe and Cu impurities show quite contrastive precipitation behaviour. Fe impurities precipitate on any type of dislocations irrespective of the rate of cooling from high temperature. More Fe atoms are accumulated on dislocations if the cooling is slow. Cu impurities need a higher supersaturation when precipitate on a Shockley or Frank type partial dislocation than on a prismatic dislocation. This results in the observation that Cu impurities at a concentration of 1 ppm precipitate on prismatic dislocations but on neither Frank partials nor glide dislocations when cooled slowly from a high temperature, while precipitate rather evenly on all the types of dislocations when cooled rapidly.

Chemistry and physics of segregation of impurities at extended defects in silicon

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Segregation of impurities at extended defects (internal or external surfaces, grain boundaries, dislocations, stacking faults) is known to affect deeply both the bulk material and extended defects properties. External and internal gettering procedures in silicon microelectronic technology are based on this knowledge, with possible future improvements which still depend on a better understanding of the chemistry and physics of these processes, here including atomistic views coming from computer simulations.
Earlier experimental studies on this topic helped in collecting the basic, macroscopic elements of the chemistry and physics of segregation processes. As an example, it was demonstrated using different spectroscopical techniques presenting lateral resolution of the order of some um or less, that impurities segregate at GB, affecting their electrical activity as barrier for majority carrier transport and recombination centres for minority carriers.
Also dislocations are credited of a strong gettering action on metallic impurities. On this assumption, mechanical damage or excess phosphorous deposition at external surfaces were used as a mean to generate high local densities of dislocations, which have been shown to work as effective and stable impurity sinks. EBIC meassurements in an extended range of temperatures, photoluminescence, cathodoluminescence and Deep Level Transient Spectroscopies were of great interest as means of detecting the influence of impurity interaction on the physical properties of these latter defects, but here still many unknowns survive. As an example, the optical emission properties of dislocations were shown to depend on impurity contamination, but it is still matter of question whether uncontrolled impurity contamination during the dislocation generation procedures plays a role.

Aim of this paper is to deal first with some general arguments concerning the equilibrium redistribution of impurities between a bulk 3D phase and an external or internal surface or a line defect, taking into account also elastic strain relief effects associated to impurity segregation and quanto-mechanical effects arising from the presence of free- and bound-electrons and holes (bound excitons, holes or electrons trapped at point defects).
Further, the reaction kinetics will also be considered, which depends on the site (substitutional or interstitial) where one reacting species sits, on the particular type of interstitial site involved (in the case of interstitial defects and impurities), on the nature (unreconstructed or reconstructed) of the extended defect and on the nature of the bond formed. By assuming that the kinetic barrier is of diffusional type, the influence of the nature of the driving force (a screened Coulombic force or a covalent binding force) on the overall process kinetics will be considered, taking into account the fact that extended defects (grain boundaries, dislocations and precipitates) could work as sources/sinks for point defects, and then, the possible influence of fast migrating point defects and, in the case of dislocations, their motion during the segregation process.
Finally, the effect of segregation on the physical properties of extended defects will be discussed in view of recent literature and of our own laboratory results.

Structural and Electrical Properties of Metal Silicide Precipitates in Silicon

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The 3d transition metals in silicon combine unusual physical properties with detrimental effects in device manufacturing. Especially, the late 3d elements cobalt, nickel and copper exhibit solid solubilities which strongly decrease with decreasing temperature and high interstitial diffusivities with small migration barriers. As a result, these impurities are mobile even under conditions of large undercooling leading to favourable conditions for precipitation.

The high quality of present day silicon materials in combination with the realisation of well - defined annealing and cooling conditions allowed to establish structural properties of silicide precipitates on the atomic scale by means of high - resolution electron microscopy (HRTEM). Deep level transient spectroscopy (DLTS) combined with appropriate modeling and quantitative simulations provided insight into the electronic structure of such defects. This paper will describe current knowledge about the interrelation of formation, atomic structure and electrical properties of silicide precipitates in silicon obtained from the combination of the above methods.

For nickel, plate - shaped precipitates consisting of two {111} planes of $NiSi_2$ with diameters between 7 and 100nm form upon quenching. High - resolution and conventional TEM show these platelets to be bounded by a dislocation with a Burgers vector of $b = \frac{a}{4} < 111 >$ which is a geometrically necessary dislocation resulting from the atomic structure of the precipitate/matrix interfaces. This dislocation is the key to understand the rapid precipitate growth as well as the deep *bandlike* states revealed by DLTS, which rapidly transform into *localized* states during internal ripening which is a phenomenon related to the metastability of the platelets.

Precursor defects to the well - known copper silicide colonies are also associated with *bandlike* states. These defects consist of copper silicide platelets which frequently give rise to the formation of a bounding extrinsic stacking fault. During internal as well as Ostwald ripening *bandlike* states are observed which are tentatively attributed to precipitate/matrix interfaces.

DISLOCATION NUCLEATION AND MULTIPLICATION AT CRACK TIPS IN SILICON

Cherlio SCANDIAN, Hamid AZZOUZI, Gérard MICHOT and Amand GEORGE

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For more than two decades, silicon has been presented as a model material, ideally suitable for studying crack tip plasticity and the brittle-ductile transition (BDT). A common view has emerged that dislocation mobility is the rate controlling mechanism which determines the critical BDT temperature at a given loading rate. However, experiments also proved that the BDT temperature is structure dependant, suggesting that dislocation formation and multiplication could take an important part in the BDT. In the present paper, emphasis is put on these latter features which are not yet fully understood.

After a short summary of BDT studies in Si, observations at crack tips will be described in more detail :

(i) In actual crystals, dislocation nucleation appeared to be highly inhomogeneous. The nature of source defects along the crack front will be examined and their efficiency discussed in terms of local loading modes and stresses on available slip systems.

(ii) In crystals containing highly perfect cleavage cracks, dislocation formation could be suppressed. In such cases, a very small number of dislocations, created on purpose from remote sources, sufficed to trigger the formation of a plastic zone as soon as they touched the crack front. The relation between the slip systems of incoming and newly formed dislocations, respectively, will be discussed.

Experimental results will be compared to theoretical models and recent numerical computations.

ON EXTENDED DEFECTS FORMATION IN SI AT COMBINED CLUSTERING OF INTRINSIC POINT DEFECTS STUDED BY IN SITU ELECTRON IRRADIATION IN A HRTEM

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The lecture accumulates last data concerning atomic mechanisms of clustering of intrinsic point defects studied by in situ electron irradiation in a high resolution transmission electron microscope (HRTEM) at room temperature. Irradiation experiments result in discovering of combined clustering of point defects strongly affected by amount of quasi-stationary concentration of point defects during irradiation, which depends on specimen thickness, irradiation intensity as well as on the condition at the surface (type of covering films).

A fundamental reason of combined clustering of point defects is an existence of energy barrier against recombination of interstitials with the extended cluster of vacancies. As a result in addition to well-known interstitial type clusters with {113} habit plane large family of extended defects on {113}- and {111} habit plane can be formed at a low and intermediate temperatures (20-700°C). At initial stages these defects can be pure defects of vacancy type. An interaction of vacancy clusters with interstitials at further stages leads to the transformation of initial defects into new type of the defects which are not vacancy or interstitial type; they are «zero» defects are characterized with very small displacement vectors and intermediate configurations of interstitials on the defect plane. Final structure of the extended defect depends on the relation between the rate of accumulation of interstitials inside cluster of vacancy type, on the one hand, and the rate of rearrangement of the atomic structure of cluster at further stages, on the other hand. It is found that the rate of rearrangement of Si-Si bonds onto intermediate defect configurations is very low at room temperature due to low energy of these configurations. For this reason high local supersaturation of interstitials, which is commonly created in Si crystal during electron irradiation, provides full transformation of the {113} defect of vacancy type into the defect of interstitial type having well-known hexagonal structure. An atomic structure evolution of the extended {113} and {111} defects elucidate the complex mechanisms of point defect recombination at temperatures range between 20-700°C depending on the dimensionality and structural configuration of initial point defect cluster as well on the amount of lattice relaxation around the one.

KINKS ON PARTIALS OF 60-DISLOCATIONS IN SILICON AS REVEALED BY A NEW TEM-TECHNIQUE

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Contributions of High Resolution (Transmission) Electron Microscopy (HREM) to the knowledge of single dislocations in semiconductors have been obtained, so far, by imagimg the dislocation in end-on orientation, i. e. with electron beam parallel to the dislocation line.
Obviously in this way kinks cannot be analyzed. On the other side details of the dislocation motion can only be settled if existence, density, mobility and pinning events of kinks are known.
Information on kinks should be embodied in plane-view images with beam perpendicular to the glide plane of the dislocation. However, in this direction columns of atoms are bent by the strain field of the dislocation so that no clear projection of the crystal structure can be expected. Nevertheless, in 1985 using a JEM 200CX we checked what can be seen.(Phil. Mag. A53 (1986) 627).
It turned out that the stacking fault ribbon betwen the two partial dislocations appears as a relatively strong contrast. This gives the possibility to attribute changes of the stacking fault width to the presence of kinks.
From the very beginning we applied this HREM technique to dislocations which were frozen in under high shear stress. This offers several benefits: those dislocations are rather staright on a weak-beam scale with an enlarged stacking fault width. Moreover, relaxing this nonequilibrium width in the microscope possibly could give insight into the kinetics of kink motion.
Geometrical analysis shows that introducing a stacking fault parallel to the crystal slab means *periodic* change of the length of atom columns. Such a change, but *nonperiodic*, is caused also by surface roughness, one of the experimental problems.
In 1995 one of the authors (H. R. K.) finished his thesis (Phys. Rev. Lett. 77 (1996) 4031) applying video-rate imaging to the relaxation of stacking faults. Evaluating difference images he could neutralize surface roughness. We so could estimate the velocity of kinks under well-known stress (due to interaction between the partials) at the chosen temperature. (As expected from weak-beam relaxation tests the 90 partial contains twice as many kinks as the 30 partial).
Various experimental conditions have been checked, two of them will be discussed. Principally the beam voltage (130kV) was chosen below the displacement limit. In one experiment a 30/90 dislocation (narrowed by the predeformation) relaxed at a temperature of 130 C where nucleation of new kink pairs can be excluded. During the relaxation period the beam was turned off, since there remain radiation influences (REDG and probably formation of pinning centers). From the velocity of the 90 partial we could calculate the migration energy W_m of kinks (W_m = 1.24 +- 0.07 eV), taking into account the kink density. The distribution of kink separations allows with Hirth`s theory to estimate the kink formation free energy $F_k$ (= 0.73 +- 0.15 eV). We feel that the agreement ($Q = F_k + W_m$) with the activation energy Q of macroscopical dislocation motion as measured by etch pits is remarkably good (Q = 2.1 +- 0.1 eV) if one uses Hirth`s theory for kink diffusion with kink annihilation.
Another standard experiment was relaxation of (widened) 90/30 dislocations at 600 C. Here the beam remained on during motion of the 90 partial so that time analysis by comparing video frames was possible. There are indications for pinning events; from waiting times one concludes an unpinning energy E_u = 2.4 +- 0.04 eV.

DISLOCATION KINK DYNAMICS IN CRYSTALS WITH DEEP PEIERLS POTENTIAL RELIEF

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The processes are reviewed of the nucleation and motion of the topological defects of ordered state (kinks), determining the dislocation mobility, and of the evolution of the dislocation structure under the stresses, being lower than the Peierls stress. The problems are analyzed of the manifold influence of point defects on the dislocation mobility. To investigate experimentally the peculiarities of the one-dimensional kink motion, being determined by the dislocation-point defects' interactions, the method of a two-level intermittent loading has been employed. The method is based on the loading of a specimen with individual dislocations by a sequence of load pulses, being separated with the "pauses" with the applied stress being much less than the one being applied during a pulse load.

The investigations are carried out with Si, Ge and bulk SiGe single crystals with Ge content up to several atomic percent, being characterized by the different ratio of the barriers, created by the point defect and by the Peierls potential. The average dislocation displacements have been measured as a function of the pulse duration, pulse separation as well as pulse leading edge. The experimental data are analyzed in the framework of a model, considering the joint interaction of numerous point defects with a dislocation.

It is shown that the Cottrell atmosphere not only determines the barriers for the kink motion, but stimulates the kink pair return to the formation centers as well as the specific mode of a kink drift along the dislocation line due to the motion in the field of random forces. This motion is determined by the step-like changes in a dislocation energy with an attachment of a point defect to the dislocation core or its detachment, being caused by a kink motion, and can lead to the nonlinearity of a kink drift or even to the localization of kinks. The experimental data obtained demonstrate the role of the nonlinear excitations in the dislocation motion over the Peierls barriers.

HYDROGEN ENHANCED DISLOCATION GLIDES IN SILICON

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The mobility of dislocations in many semiconductors is sensitive to the electrical properties of the crystals, which is considered to be owing to the presence of band gap states associated with dislocations. Hydrogen incorporated into semiconductors reacts with various kinds of defects and changes their electronic properties. One may therefore expect that the incorporation of hydrogen into the crystal would affect the dislocation mobility as well. Actually, Haasen et al. [1] reported that mechanical softening of silicon was induced by irradiating of the crystal with hydrogen plasma. However, there has been no direct experiment to study the effects of hydrogen on the velocity of individual dislocations. This paper reports on our recent experiments showing that the incorporation of hydrogen atoms quite remarkably enhances the mobility of 60° dislocations in Si [2]. Moreover it has turned out that a pre-hydrogenation treatment is essential to this enhancement effect to occur.

The samples used were cut from a P-doped n-type FZ-Si (n = $5.9\times10^{14}cm^{-3}$) crystal into rectangular plates ($2.7\times15\times0.4mm^3$) with the longest dimension parallel to the [123] direction. After dislocation loops were introduced by four-point bending at a distance about 100μm from a scratch, the sample was subjected to the first etching. The sample was remounted on the bending stage without loading and was irradiated with RF-generated hydrogen plasma for 1 hour at 540 °C (pre-hydrogenation treatment). Then, the sample was loaded at various temperatures to extend the dislocation loops under hydrogen plasma. The second etching determined the dislocation velocity.

It was observed for the first time that the dislocation velocity was promoted under hydrogen plasma by a factor of 10 to 100 in the temperature range of 390 - 480 °C. The activation energy and the prefactor were both reduced to 1.2 eV from 2.2 eV and to 2m/s from 8×10^5m/s, respectively. Thus, the effect was only observed below a certain temperature. This phenomenon resembles the radiation enhanced dislocation glides (REDG) induced by electronic excitation. However, we confirmed that the enhancement effect is attributed not to plasma light which may induce the REDG effect, but to hydrogen itself incorporated into the sample. An experimental evidence was that the sample irradiated with plasma of nitrogen, instead of hydrogen, did not show the enhancement of the dislocation velocity. Another support was provided by the fact that the use of an opaque cover to cut the light from hydrogen plasma still yielded the enhancement of dislocation velocity.

As far as the sample had been subjected to the pre-hydrogenation treatment, the effect was observed even if the sample was not in hydrogen plasma during loading. Conversely, if the pre-hydrogenation treatment was omitted, the dislocation velocity was not promoted at all. These facts indicate that the pre-hydrogenation treatment, rather than hydrogen environment during loading, is essential to this effect. It is highly possible that hydrogen atoms are accumulated in dilated regions and form a dense Cottrell atmosphere around the dislocation lines at sufficiently low temperatures (in the present study, 480 °C below which the enhancement effect can be observed). We further speculate that hydrogen atoms in the Cottrell atmosphere react with kinks on the dislocation lines to lower their formation energy by an amount of the binding energy between a kink and hydrogen, and as a consequence enhance double kink formation.

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DISLOCATION MOBILITY IN SILICON FROM ATOMIC CORE TO MICRON SCALE

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It is commonly accepted that dislocation motion in Si is controlled by the kink mechanisms. Based on this notion, the well known kink diffusion model leads to a simple rate equation describing temperature and stress dependence of dislocation mobility. However, a detailed analysis of the available experimental data shows that this simple approach fails to account for the realistic complexity of dislocation motion, both at the core level and on a larger, mesoscopic scale. We propose a quantitative theory of conservative dislocation motion in Si that bridges these distinct length and time scales. This multiscale theory contains no adjustable parameters and combines accurate atomistic calculations of the core energetics and mechanisms with kinetic Monte Carlo simulations of micron scale dislocation behavior. The theory provides a close description of the observed complexity of dilsocation behavior in Si and, in addition, suggests several specific experiments to test its predictive capabilities.

GROWTH AND PROPERTIES OF BULK SINGLE CRYSTALS OF GaN; ROLE OF DEFECTS

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Most of GaN-based devices consist of epitaxial layers of III-V nitrides with dislocation densities as high as 10^{10} cm^{-2}. The defects which are inherent to the growth of GaN epilayers are caused primarily by large difference between the lattice parameters and the coefficients of thermal expansion of GaN and available substrates. An explanation of high efficiency of blue and ultraviolet light emitting diodes in such highly defective semiconductors remains unclear. Moreover, a number of parameters characterising physical properties of GaN is significantly modified by presence of the defects.

High Pressure Research Center is the only place where monocrystals of GaN in form of platelets with 100 mm^2 surface and concentration of dislocations below about 10^5 - 10^6 cm^{-2} are synthesized. It requires application of nitrogen pressures in the range of 1.5 GPa and temperatures ~1500°C. The described GaN bulk crystals, when undoped, represent highly conductive material with electron concentration achieving 10^{20} cm^{-3}. Growth procedure consisting in use of a Ga-melt with Mg impurity leads to highly resistive materials. The obtained GaN crystals are used as substrate in processes of homoepitaxial growth of almost perfect structures.

In this talk it will be discussed a role of native defects (N- and Ga-vacancies and/or O- and Mg-impurities) in determining optical and electrical properties.

EXTENDED DEFECTS IN GaN

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Wide band gap semiconductor materials have attracted considerable interest for applications in optoelectronics, high temperature and high power microelectronics devices. Out of three widely studied semiconductor materials such as ZnSe, SiC and GaN, the latest one is the most attractive due to its direct band gap. Despite recent impressive improvements in the quality of GaN-based materials the best currently available material used in blue lasers is still highly defective, with thin film structures having dislocation densities in the 10^8 to 10^9 cm^{-2} range. These dislocations are often arranged in small-angle grain boundaries. For the layers with higher residual strain twin-like grain boundaries are formed.

Another type of the deleterious defect in GaN are nanotubes and pinholes. The origin of these defects cannot be explained as hollow-core screw dislocations, since the measured and calculated Burgers vectors differ at least one order of magnitude. It will be shown that in GaN two related types of defects can be formed: nanotubes along the *c*-axis and pinholes in the subsurface area. Both these defects start with V shaped facets on{101} polar planes and can be originated by various kinds of inhomogeneities or impurity clusters. Formation of these defects is caused by the strong dependence of growth rate on different crystallographic directions.

The quality of currently available GaN material is limiting the performance of devices. In order to control the defect formation, it is essential to better understand their nature. Transmission electron microscopy was applied to explain the atomic structure of defects that will be characterized during this presentation.

Structural characterization of extended defects in GaN epilayers and AlN/GaN heterostructures by Transmission Electron Microscopy

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Recently, stirred by many applications in optoelectronics, GaN and its alloy with AlN and InN have attracted many attentions. However during the eighties, due to a lack of an adapted substrate and difficulties in p-type doping, GaN was considered as an inadequate material for optoelectronics and II/VI materials were preferred. The interest in III/V nitrides exploded in 1993 with the realisation of the first blue diode by Nakamura, followed soon by the realisation of a blue laser diode. Time is now at device optimisation and basic understanding.

Basic research aims are (i) to understand how can extended defects in GaN can or cannot affect light emission and (ii) how can their number can be reduced. One of the first step in such searches is to identify the extended defects present in these layers and Transmission Electron Microscopy is one of the most powerful tool to do so.

In this talk, we will review the different extended defects we have observed in wurtzite GaN layers grown by MBE or by MOCVD on (0001) sapphire. It will be shown that polarity and III/V ratio greatly influence the type of defects present in these layers.

Observations of AlN/GaN heterostructures (superlattices and quantum dots) will be also quickly presented.

CL AND TEM STUDY OF OPTICALLY ACTIVE DEFECTS IN GaN AND AlGaN EPILAYERS GROWN ON SAPPHIRE

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In the last few years GaN and related nitrides have shown to be reliable for the production of optoelectronic devices in the ultraviolet energy region [1]. Further, due to the large direct bandgap and excellent thermal conductivity, even in microelectronics GaN and related nitrides are now competing with GaAs or InP based MODFETs, SiC based FETs, MESFETs and HEMTs. Nevertheless, despite the excellent results, several problems connected to the comprehension of the physical mechanisms at the basis of optical and electrical properties of both materials and devices are still open. As an example, the large lattice mismatch and different thermal expansion coefficients inside the structures and/or with the most common substrates, are responsible for defect generation, residual strain, compositional inhomogeneities, additional optical transitions etc..

In this paper, low temperature (5 K) spectrally resolved cathodoluminescence (SCL) and high resolution transmission electron microscopy (HREM) investigations will be employed to correlate optical and structural properties of undoped and differently doped GaN and AlGaN epitaxial layers. As for undoped GaN, it will be shown that an additional UV line at about 3.43 eV can be correlated to the occurrence of stacking faults (SFs), independently on the type of substrates and of the growth techniques employed. The presence of the line will be explained by a model based on the concept of excitons bound to SFs that form a quantum well of cubic material in the wurtzite lattice of the layer. The effect of different doping levels on crystal defects and optical transitions in both p- and n-type GaN grown by MBE on (0001)Al2O3 will be also discussed. Concerning AlGaN epilayers, the results on both undoped and Si doped layers grown by MBE on (0001) oriented sapphire with an Al molar fraction between 0.6 and 1 will be presented. The influence of dopant on the onset of additional optical emissions and their temperature and excitation power dependence will be first discussed. Further, depth resolved SCL spectra showing a possible Al concentration variation from the top surface to the epilayers interface will be discussed in terms of the presence of a cubic phase and residual strain as suggested also by HREM investigations. SCL and absorbtion spectra and HREM investigations vs Al concentration, carried out to study the correlation between the onset of indirect band gap transitions and the presence of a predominant cubic phase for Al molar fraction larger than 0.5, will be also shown. Finally, the broadening of the SCL NBE emission as a function of the composition and its correlation with the increasing cubic phase/exhagonal phase ratio will be discussed by comparing our experimental results with a model from the literature [2].

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INTERACTION OF OXYGEN WITH DISLOCATIONS IN GaN

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Abstract

First principles calculations are used to investigate the structure and electronic properties of dislocations in GaN. It is found that both cores are reconstructed without any deep states. The atoms comprising the wall of the core of the screw dislocation possesses heavily strained bonds and there is a reduction in line energy when the first shell of Ga and N atoms is removed leading to a screw dislocation with a small open core. The interaction of oxygen with the cores of both dislocations is considered and it is found that the impurity has a strong tendency to be bound by Ga vacancies leading to three types of defect trapped in the strain field. We suggest that the most stable defect leads to a poisoning of growth centres on the walls of nanopipes.

Oxygen and carbon precipitation in multicrystalline solar silicon

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Multicrystalline silicon grown by directional solidification and polycrystalline RGS silicon are low cost materials for photovoltaic applications. The properties of solar cells made from these materials are mainly determined by dislocations, impurities, and small clusters of atoms or precipitates. Oxygen and carbon are the main impurities and thus play a major role.

Oxygen is known to affect the conversion efficiency of solar cells. The impurity can form a variety of defects that affect the electrical behavior differently. Clusters of a few oxygen atoms and various sizes and crystal structures are observed for larger SiO_2 precipitates. Well known defects are also the Thermal Donors which are clusters of a few oxygen atoms and the New Donors that have been connected with SiO_2 precipitates. In addition, oxygen can precipitate at grain boundaries and dislocations and change their electrical behavior.

The defects can have an impact on the diffusion length, the mechanical strength and on the properties of the pn - junction if they are large enough to penetrate the space charge region of a solar cell. Furthermore, oxygen precipitates are efficient gettering sites and can reduce the efficiency of the phosphorous and / or aluminum gettering steps during solar cell processing. In the presence of carbon the precipitation behavior of oxygen can be changed. In addition, carbon also precipitates and can form detrimental SiC precipitates. The evolution of both oxygen and carbon defects depends very much on the thermal history of the material and every thermal step between crystal growth and solar cell process has to be considered.

In this paper results are summarized that demonstrate the important role of oxygen - induced defects in multicrystalline silicon. P-type mc - cast silicon ingots and RGS ribbons with various concentrations of oxygen (1 - 20 ppm) and carbon (0.05 - 50 ppm) have been used for the investigations. The grain sizes were on average 1 cm or 0.5 mm, respectively, the average dislocation densities varied between 10^5 -10^7 cm^{-2}.

As-grown and annealed specimens were electrically characterized by resistivity, C-V, and DLTS measurements. The behavior of oxygen and carbon was studied by FTIR. The distribution of the dissolved elements was determined by mapping the entire specimen. The chemical composition of particular bulk defects and precipitates was investigated by EDS and scanning Auger spectroscopy, the distribution and morphology of grain boundaries, dislocations and precipitates by TEM, HREM and SEM.

Furthermore, in a systematic study the oxygen and carbon precipitation in polycrystalline silicon has been investigated under defined conditions. Annealing experiments were carried out between 300 - 1200 °C and the time and temperature dependence studied and compared with the behavior of oxygen and carbon in Cz - silicon. It could also be shown that the oxygen precipitation process can be accompanied by the formation of New Donors. The position and the height of the maximum concentration depends mainly on the oxygen concentration and to some degree on the carbon concentration as well. The donors are related to the formation of oxygen precipitates of various structures and morphologies.

Because of the technical importance of the oxygen precipitation process, a numerical program based on recent precipitation theories using rate equations supplemented by a Fokker-Planck type equation has been developed that allows one to simulate the precipitation process and to determine the size and density distribution of the precipitates for any thermal treatment. The numerical results are compared with the experimental investigations on mc - and RGS silicon that has been processed under various conditions. The aim of this approach, to predict the size and density of oxygen - induced defects for any sequence of thermal treatments that a material experiences, has been achieved with sufficient accuracy.

RECOMBINATION - ENHANCED MICROPRECIPITATE FORMATION IN LPE GaAs STRUCTURES

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Variation of luminescence spectra, electrical characteristics and deep level defect spectra in LPE GaAs:Si structures in nonequalibrium condition (injection, photoexcitation, small doze radiation) was investigated. Electron-microscopic studies have been done as well.

Experimental results were analyzed and the theoretical model for transformation of defects in LPE GaAs epitaxial structures doped by Si was proposed. It is shown that the nonmonotonic kinetics of the luminescence intensity variation in these structures in unequlibrium conditions can be described well by recombination - stimulated dissociation of simple impurity -intrinsic defect complexes, followed by diffusion of movable intrinsic defects and their coagulation into the microprecipitates acting as nonradiative recombination centers.

The theoretical model of this complete processes have been created, where we attempted to describe the dynamics of the microprecipitate formation and growth in GaAs structures with the use of the theory of condensation of excitons into electron-hole droplets. The theoretical model is used to explain the observed exponential rise of the luminescence intensity of GaAs:Si structures and the subsequent fall of the radiation intensity in accordance with the law $W \sim (at)^{-2/3}$, and also to calculate the defect formation efficiency representing the process of recombination - stimulated dissociation of simple impurity - intrinsic defect complexes.

Then the numerical calculation of the kinetics of GaAs:Si luminescence variation in nonequalibrium condition have been done. The comparison of the numerical result with experimental kinetics of the GaAs LED emitting power degradation give possibility to explain the complicated luminescence kinetics and it dependencies from temperature and injection current, as well as to estimate the diffusion coefficient for intrinsic lattice defects, apparently interstitial Ga atoms, and to prove that the processes of these interstitial atom diffusion in GaAs layers is not recombination - enhanced one.

We have shown that such transformation defect processes limit the service life and radiation stability of optoelectronic materials and light-emitting devices.

Formation of dislocations in InGaAs/GaAs heterostructures

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Heterostructures of $In_xGa_{1-x}As/GaAs$ are very important for future applications since they have potential use for such optoelectronic devices as semiconductor lasers, resonant tunneling diodes, infrared detectors. Lattice parameter of $In_xGa_{1-x}As$ depends on the content of indium. The difference between lattice parameters of $In_xGa_{1-x}As$ and GaAs is a reason for the occurance of lattice misfit. Significant misfit between crystalline lattice of $In_xGa_{1-x}As$ and GaAs causes the formation of dislocations in a heterostructure. This process depends on thickness of $In_xGa_{1-x}As$ layers. Summarizing, the structural perfection of $In_xGa_{1-x}As/GaAs$ heterostructure depends on indium content in $In_xGa_{1-x}As$ alloy and the thickness $In_xGa_{1-x}As$ layers [1].

$In_xGa_{1-x}As/GaAs$ heterostructures of various thicknesses of $In_xGa_{1-x}As$ layer and various indium content were grown by means of molecular beam epitaxy on a (100)-oriented GaAs semi-insulating substrate in a Riber 32p setup. Structural perfection of heterostructures were determined using transmission electron microscopy and X-ray diffractometry.

The purpose of this paper is to understand how the geometry of heterostructure and the indium content in $In_xGa_{1-x}As$ layer influences the lattice perfection of heterostructure. From the wide range of thicknesses and contents only those having practical application in devices were selected.

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Crystalline Defects as Enhancement and Limits to Microminiaturization.

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Abstract.

This brief review monitors the use of small crystalline defects, such as dislocations, in the design of diodes, bipolar and field effect transistors along the microminiaturization trend in electronics. In the early 80`s, use of single dislocations as electronic elements on a semiconductor chip was seen as a viable alternative to make the smallest transistor. Successful development of low dimensional electronic devices significantly reduce the necessity for potential use of linear defects. At the same time attention should be paid to dislocations affecting wafer processing.

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FROM POINT TO EXTENDED SELF–INTERSTITIALS IN SILICON: A TIGHT–BINDING MOLECULAR DYNAMICS STUDY[1]

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We discuss the coalescence of self-interstitials in silicon to get insight on the mechanism of nucleation of extended defects, like {311}'s, rodlike structures and dislocation loops. In particular, we will address the following problems:

1. Which are the basic building blocks for the formation of self–interstitial extended defects ?
2. What about the stability of extended defects ?
3. Which is the growth mechanism of such structures ?

Our investigation is based on large–scale tight–binding molecular dynamics (TBMD) simulations.

The basic idea is to apply TBMD to simulate ground–state, as well as finite–temperature properties. In the former case, we will investigate the energetics of formation, the stability, and the atomic configuration of the defect complex by total-energy calculations. Finite–temperature simulation will be next applied to study the interaction features among isolated interstitials and extended defects.

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RECOMBINATION-ENHANCED DISLOCATION MOTION IN SiGe AND Ge

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The phenomenon that dislocation glide is enhanced during carrier injection into a crystal by forward biasing or by laser irradiation is well known as recombination enhanced dislocation motion (REDM). Quantitatively analyses have been reported in Si, GaAs and other several semiconductor materials. However, in Ge only a negligible effect is known caused though by low-voltage electron injection. It is also interesting to study REDM in alloy semiconductors. We investigated the REDM in Ge and SiGe alloys with *in-situ* observation of dislocation glide in Ge and SiGe alloys in a high voltage transmission electron microscope (HVTEM).

The specimens prepared from Ge and Si-5at%Ge alloy crystals were deformed by using a heating tensile stage in an HVTEM at elevated temperatures in the range 420 - 660°C and 610 - 840°C, respectively. The motion of dislocations under an effective stress of up to 24 MPa was observed in-situ and recorded on video tapes. In both materials dislocations moved easily during the in-situ TEM observation and their velocities decreased with decreasing the electron beam current. Compared with the results on dislocation glide in the dark, the dislocation velocities were found to be enhanced at low temperatures. The glide activation energy of 60° dislocations during the in-situ observation was estimated to be 1.5 eV in Si-5at%Ge, similar to that obtained with electronirradiation or illumination in Si. On the other hand, the glide activation energy of dislocations turned out to be only 0.7 eV in Ge.

REDM is thought to be caused by nonradiative carrier recombination at dislocations. The energy released by the recombination is converted to a lattice vibration and can help either double kink formation or kink migration in the dislocation glide process. It has been argued previously that the injected high-density carriers as in the HVTEM attribute mainly to recombination-assisted kink formation rather than as recombination-enhanced kink migration. Inthis case, the observed beam-induced reduction of activation energy can be understood as the kink formation energy. In this model, he present results seem to suggest that the kink formation energy 1.0 eV in Ge is even larger than that 0.6 eV in Si, whereas the kink migration energy is considerable smaller than in Si.

DEFORMATION OF SINGLE CRYSTAL 4H- AND 6H-SiC

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The wide band-gap semiconductor, SiC, is recently a focus of much attention because of its applications in high-power, high-frequency electronic devices that can be employed at high temperatures. In this talk, we shall consider some deformation studies on single crystals of two SiC polytypes: 4H and 6H. The deformations were conducted under compression on single crystals of 4H and 6H-SiC oriented for single slip. The yield stress of these two polytypes were determined as a function of temperature and strain rate, and the dislocation structure in the deformed crystals were studied by transmission electron microscopy (TEM) on thin foils parallel to the slip planes of the deformed crystals. From the generated data, activation parameters for dislocation glide in 4H- and 6H-SiC were evaluated that shed new light on generation and glide of dislocations in hard materials such as SiC.

POSITRON ANNIHILATION AT DISLOCATIONS AND RELATED POINT DEFECTS IN SEMICONDUCTORS

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Extended studies of the defect spectrum formed during plastic deformation of semiconductors have been carried out by means of positron lifetime spectroscopy. So far, dislocations have been mostly treated in positron annihilation as simple rows of vacancies. However, the trapping of positrons in extended defects is more complex than for vacancies. A more sophisticated approach takes into account that the undisturbed dislocation line, which is free of defects such as kinks, jogs, or associated vacancies, acts only as a weak trap for positrons. The interaction of the positron with dislocations can be understood in terms of a two–stage cascade process. The undisturbed dislocation line is a precursor trap for the positron capture in a deeper trap. Such deep traps are related to vacancies bound to the dislocation. The open volume of kinks and jogs is not much different compared to the undisturbed dislocation, and they are consequently no deep positron traps. The transition to the deep level is very fast, so that thermal detrapping of positrons from the shallow level may be neglected for neutral dislocations. The annihilation rate (the reciprocal positron lifetime) of the defect–free dislocation line is not very different from the bulk annihilation rate in the bulk of the semiconductor. A solution of the set of rate equations for the trapping in dislocations can be easily given, if the direct trapping in dislocation–bound vacancies is neglected. The negative charge of dislocations in n–type semiconductors leads to the formation of extended shallow Rydberg states. For simplicity, the same shallow positron state as for uncharged dislocations may be assumed, but the detrapping rate cannot be neglected anymore.

It is rather difficult to separate in positron lifetime spectroscopy the dislocation signal from the contributions of point defects generated via dislocation motion. In addition to dislocation–bound defects, there are other positron traps, such as vacancies and vacancy clusters. A further complication arises with the appearance of point defects acting as shallow positron traps. It is hardly possible to separate reliably more than two defect–related components from the decomposition of positron lifetime spectra. More information can be obtained from the measurement of the positron lifetime as a function of the sample temperature in conjunction with annealing experiments. Peculiar features in the temperature–dependent average positron lifetime around 100 K may be due to the presence of a metastable defect configuration, which is connected with the strain field in the sample after compression.

A high positron lifetime component of approximately 500 ps found practically in all plastically deformed semiconductors indicates the presence of open–volume defects which are distinctly larger than monovacancies. They are identified as vacancy clusters, which can already be formed at rather low deformation temperatures. The mechanism of the formation of the clusters does not involve vacancy diffusion, but is connected with the dragging of jogs along screw dislocations. The concentration of generated defects depends on the number of activated slip systems. It can be related to a different density of jogs formed by the intersection of dislocations.

THE RELATION BETWEEN MISFIT DISLOCATIONS STRUCTURE AND *PL* IN $Si_{1-x}Ge_x$/Si(100) HETEROSTRUCTURES

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The dislocation structure and photoluminescence (PL) of partially relaxed $Si_{1-x}Ge_x$ layers on Si(001) substrates were studied to clarify the contribution from dislocations localized in different regions of the heterostructure (the SiGe layer, the substrate, and the interface) to the dislocation-related PL lines. The D1 and D2 lines were found to be related to the misfit dislocation network. It was supported that the products of dislocation reactions at dislocation intersection points in the misfit dislocation network are responsible for these lines. The D4 line is shifted from the position expected from the known dependence of the D4 line energy on the alloy composition. This was supposed to be stipulated by the elastic strain in the layer.

CORE STRUCTURES OF SCREW DISLOCATIONS FORMING SQUARE GRIDS IN SI: MOLECULAR DYNAMICS STUDY

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Up-to-date UHV wafer bonding technique allows to form covalent bonds between atoms of (001)Si surfaces brought into contact. If the surfaces are properly cleaned, bonds are formed even at room temperature, that is no subsequent thermal treatment is needed. Inavoidable rotational misorientation between the bonded (001)Si wafers introduces bond distortions which relax to form a square grid of a/2<110> screw dislocations, identical with a low-angle twist boundary. Unlike misfit dislocations accomodating difference in lattice parameters in heteroepitaxial systems, the interface dislocations in (001)Si/Si system occur without any bulk plastic deformation in the bonded wafers. They likely result from spontaneous rearrangment of bonds between atoms in the interface region and localization of bond distortions near the dislocation lines. Despite a lot of experimental data have been already accumulated as for the screw dislocations, actually a little is known about atomic structures of their cores. According to HREM observations, the screw dislocations do not split into partials. Spreading resistance measurements revealed also that such square grids of screw dislocations are electrically active (directly or by trapping oxygen) and responsible for positively charged interfacial states, with the positive charge density increasing as the misorientation of wafers (that is the dislocation density) increases.

It is suggested in this study that core structures of screw dislocations in square grids may differ from those of isolated dislocations, depending on whether both sets of parallel dislocations forming a grid lie in one (001) plane (single-plane model) or in two neighbouring (001) planes separated by a fourth of the lattice parameter (double-plane model). Such situation becomes possible for the single-plane model since in this case two orthogonal directions [110] and [$\bar{1}$10] are structurally inequivalent. One of them coincides, in particular, with the direction of dimer rows on reconstructed (001) surfaces of the bonded wafers. To analyse core structures of the screw dislocations and especially their intersections, where the maximum structural disorder is expected, classical molecular dynamics (MD) simulations with the empirical many-body potentials of Tersoff and Stillinger and Weber were performed. A dislocation grid comprising two pairs of orthogonal screw dislocations was introduced into a large cluster of atoms using linear elastic displacements modified to take into account geometrical nonlinearities corresponding to the scheme of Euler. It was shown that the symmetry of initial atomic configurations can be improved if the field of displacements in Euler's coordinates is used.

MD studies of the double-plane model showed that the core structure of all dislocation segments is similar to that of a shuffle-set screw dislocation with the (111) glide plane. In addition, it was found that at the points of dislocation intersections all atoms are four-fold coordinated, however with high angular distortions of bonds. In the case of the single-plane model MD simulations revealed that cores of some dislocation segments possess complex atomic structure. The core atoms are no longer four-fold coordinated, however, the perfect coordination can be restored by forming new bonds along the dislocation line. The resulting bonding topology resembles the core structure of a dipole of reconstructed 30° dislocations with the (111) glide plane. Models of reconstruction for intersections of orthogonal screw dislocations were also proposed.

STRUCTURAL AND ELECTRONIC PROPERTIES OF HIGH-ENERGY, DISORDERED GRAIN BOUNDARIES IN INTRINSIC SEMICONDUCTORS

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The atomic and electronic structure of representative high-energy (twist) grain boundaries in Si and C is theoretically investigated by a tight-binding model Hamiltonian. The interface atomic structure is obtained after high-temperature annealing and quenching, simulated by constant-(NPT) molecular dynamics, and final relaxation with a second-derivative-based gradient algorithm. Electronic properties are studied in terms of the bond-length and bond-angle disorder, localization of edge and tail states by disorder and coordination defects.

Useful insights in the correlation between atomic and electronic structure are obtained by comparing the same grain-boundaries in Si, a prototype of tetrahedral semiconductors, and C, which displays a richer bonding allotropy.

Molecular dynamics simulations show that the equilibrium atomic structure of high-energy grain boundaries in silicon is similar to that of bulk amorphous silicon and contains coordination defects. The corresponding electronic structure is also amorphous-like, displaying gap states mainly localized around the coordination defects, where large changes in the bond-hybridization character are observed. We propose that such coordination defects in disordered high-energy grain boundaries are responsible for the experimentally observed gap states in polycrystalline Si.

By contrast, high-energy grain boundaries in diamond tend to relax the excess interfacial energy by a combination of structural and bonding disorder. The large fraction of sp^2 bonding thus arising introduces π-π^* bands in the perfect-crystal bandgap. The resulting electronic density of states is, however, not strictly graphitic because of the strong localization of the π bands at distorted sp^2 dimers. By combining structural and electronic analysis, we show that some degree of conduction by hopping mechanisms could be in principle allowed.

Specific features to experimentally identify effects from the disordered grain-boundary structures, such as EELS spectra, are also discussed.

Ge/Si (111) INTERFACE MISFIT DISLOCATION NETWORK MODELING

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Lattice mismatch induces misfit dislocations at the interfaces between Ge layers on Si samples for layer thickness exceeding a critical value h_c. We provide results from computer simulations [1] of the hexagonal misfit dislocation networks for Ge/Si(111) structures and, for comparison with the literature, for parallel dislocation arrays in case of Ge/Si(001) layers.

For the Ge/Si(111) misfit dislocation network a splitting into partials is considered as predicted by the experiments [2,3]. The calculations are carried out by using the anharmonic bond charge model [4] and, for completeness, the Stillinger-Weber potential. Locally stable atomic configurations are generated by using a steepest descent approach, including up to 30,000 atoms in the basic cell. The calculations predict as energetically most favorable network configuration the split dislocation structure deduced by Hansson, Ernst and Bauser [2] from their HREM investigations. The experimentally also observed alternative structures [3] turn out less favorable due to the large number of dangling bonds in the misfit dislocation cores. They may get similar energies as structure [2] if suitable saturation of the dangling bonds can be achieved.

Proper inclusion of stacking fault and surface reconstruction energies predicts a critical thickness of about 0.66 nm in case of the structure from [2], while for the structures from [3] 1.0 nm is estimated by assuming misfit dislocations with unreconstructed cores.

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THE INTERACTION OF OXYGEN WITH OPEN SCREW AND THREADING EDGE DISLOCATIONS IN GAN

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Local density functional methods are used to examine the core structure and oxygen segregation at edge and screw dislocations in GaN. Both these types of dislocation were constructed using elasticity theory. In the impurity free edge dislocation the core structure is similar to that found for the (10-10) surface leading to a gap free from deep levels. However, we find that it is energetically favourable for defects, such as the gallium vacancy oxygen complex to be trapped at the core region of the threading edge dislocation. It has been suggested that such defects are correlated with the yellow luminescence band in GaN. The screw dislocation with a filled core possesses strained states but a screw with an open core is free from gap states. Oxygen has a strong tendency to migrate to the (10-10) surface. Theory identifies another gallium vacancy oxygen defect to be particularly stable and electrically inert. In growing crystallites it is suggested that these defects segregate to the surfaces where grains meet. As crystalline growth proceeds the area of the cavity surface contracts leading to an increased defect density that inhibit further growth and prevent the filling-in of the cavity thus creating a nanopipe.

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A NEW MODEL FOR PARTIAL DISLOCATION SOURCE IN SEMICONDUCTORS

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Partial dislocations nucleation and multiplication in III-V semiconductor compounds are usually ascribed to the differences in mobility between α and β partials. These differences in mobility increase when temperature decreases, so that the contribution of twinning to the deformation mechanisms becomes important, in these compounds, for high stresses and low temperatures.

Starting from TEM observations of plastically deformed InSb under high stresses and hydrostatic pressure at room temperature, showing the multiplication of α as well as β partial dislocations, a model for partial dislocation multiplication is proposed. This model does not rely on the difference in α and β partial dislocation mobilities but on the formation of Lomer-Cottrell sessile dislocations issued from dislocation dipoles. Conditions for operation of such sources are discussed and compared to experimental evidences.

STACKING FAULT ENERGIES OF TETRAHEDRALLY COORDINATED CRYSTALS

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The intrinsic stacking fault energy has been determined by electron microscopy from the width of the extended dislocations for nineteen tetrahedrally coordinated crystals: three with the diamond structure, ten with the zincblende structure and six with the wurtzite structure (measurements have been made by the present authors for seven crystals). The obtained stacking fault energies range from a few mJ/m^2 to $300mJ/m^2$. The reduced stacking fault energy (RSFE:stacking fault energy per bond perpendicular to the fault plane) has been correlated with various material parameters. A correlation is found to exist between the RSFE and the charge redistribution index and also between the RSFE and *c/a* ratio of the wurtzite structure (for many of the diamond and zincblende crystals, the wurtzite structure has also been reported as a metastable phase). The implication of the correlations has been discussed from the point of the relative stability of the crystals between the cubic structure and the hexagonal structure; the stacking fault energy of a crystal signifies the free energy difference between the two structures because the stacking fault region takes the other structure different from the matrix.

PLASTICITY OF III - V COMPOUNDS AT LOW TEMPERATURES

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Plastic deformation of GaAs, InP, and InSb under hydrostatic confining pressure has been performed in the temperature range 77 - 500K. Observations of slip lines indicate that $\frac{1}{2}<10\bar{1}>$ dislocations cross-slip from the {111} glide planes[1,2]. TEM observations reveal many screw dislocations left in the deformed specimens[1,2]. The temperature dependence of the critical shear stress τ_c around 300K is weak, producing a hump in the τ_c - T curve[2]. These observations seem to contradict the commonly accepted understanding that dislocations in III - V compounds are dissociated into two Shockley partials in the glide set planes[3]. The activity of nondissociated screw dislocations, which probably move in the shuffle set planes and cross-slip, might be responsible for the plastic deformation of these III - V compounds at low temperatures.

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DISLOCATION VELOCITIES AND MECHANICAL STRENGTH OF BULK GeSi CRYSTALS

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Semiconductor alloy GeSi is a complete solid solution system with a diamond cubic structure. The lattice constant of these two elements differ by 4% and the solid solutions follow Vagary's Law closely. Since the mechanical behaviour of Si and Ge is well understood on the basis of kinetic properties of dislocations, GeSi alloy is quite suited for the basic study to extract unique dislocation process in such solid solution. This paper reports the dislocations mobilities and mechanical strength of bulk crystals of $Ge_{1-x}Si_x$ alloys in the whole composition range $0 < x < 1$ grown by the of the Czochralski method.

The velocities of dislocations were measured by the etch pit method. In the GeSi alloys of the composition range $0 < x < 0.08$ (Ge-rich side) the dislocation velocity decreases monotonically with increasing Si content, reaching about one of seventh of that in pure Ge at $x = 0.08$ in the temperature range 450 - 700 °C and the stress range 3 - 24 MPa. Contrarily, in the composition range $0.94 < x < 1$ (Si-rich side) the dislocation velocity first increases and then decreases with increasing Ge content in the temperature range 750 - 850 °C and the stress range 3-30 MPa. The dislocation velocity for the Ge content $(1 - x) = 0.004$ (the Si content $x = 0.996$) is higher than that in pure Si. The velocities of dislocations in the GeSi alloys of the above Ge-rich and Si-rich compositions are expressed by an emprical equation of functions of the stress and temperature well known in Ge, Si and other semiconductors.

The mechanical strength was investigated by compressive deformation tests. The stress-strain curves in the yield deformation of the GeSi alloys of the composition range $0 < x < 0.4$ (Ge-rich side) are similar to those of pure Ge and are temperature-sensitive at temperatures lower than about 600°C. However, the yield stress becomes temperature-insensitive at higher temperatures and increases with increasing Si content. The stress-strain curves of the GeSi alloys of the composition range $0.94 < x < 1$ (Si-rich side) are similar to those of pure Si at temperatures 800 - 1000°C and the yield stress increases with decreasing Si content down to $x = 0.94$. The yield stress of GeSi alloys seems to show the maximum around $x = 0.5$ and to depend on the composition as proportional to $x(1 - x)$.

The flow stress of GeSi alloys at an elevated temperature has an athermal component that is absent in elemental or compound semiconductors and gives rise to the alloy hardening. Such athermal component of the flow stress is thought to originate in built-in stress fields related to local fluctuation of the alloy composition and also dynamic development of solute atmosphere around dislocations.

STRUCTURE AND CLIMB OF FAULTED DIPOLES IN GaAs

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Three types of dislocations, α, β and screw dislocations are known in sphalerite and wurzite compound semiconductors and exhibit quite different dynamic properties and impurity effects. However, the micro-structural understanding on them has not yet been established even using high resolution electron microscopy (HREM), since the dislocations are unstable during the observation. Faulted dipoles are generated following the interaction of dissociated dislocations having opposite ***b*** moving on parallel slip planes and are stable, which is a candidate for the structural understanding of the extended defects. This paper reports the micro-structure of the faulted dipoles and climb of the partial dislocations in GaAs observed using HREM.

An HREM image of the Z-type faulted dipoles in GaAs is shown in Fig. 1. The fault consists of three intrinsic stacking faults with two stair-rod dislocations and two 90° Shockley partial dislocations at both ends. The convergent beam electron diffraction technique revealed that the partial dislocations at the top part of the defect to be β-type and those at the bottom of the defect to be α-type. There is no difference in the core structure of the α and the β dislocations of stair-rod and Shockley type, nor in the associated stacking fault widths. The stacking fault energy was estimated to be 57 ± 17 mJ/m^2.

Strikingly, in the stacking fault between the stair-rod dislocations, white spots split into paired small white spots. Normally, Ga and As dumbbell atoms are observed as white spots in HREM images in the resolution limit of a microscopy. This shows that some atomic arrangement of the cetral stacking fault differs from that of the other stacking faults.

After prolonged e-irradiation for observation, 90° Shockley partials of α and β type forming part of a faulted dipole climbed through absorption of interstitials. This means that the dislocation climb initiates with the formation of perfect dislocation loops located on the partial dislocations.

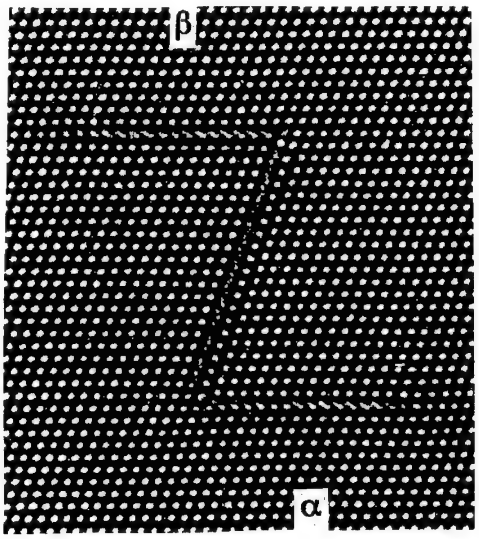

Fig. 1. HREM image of a faulted dipole

MECHANISMS OF ENERGY DISSIPATION DURING DISPLACEMENT-SENSITIVE INDENTATION IN SINGLE CRYSTALS OF SEMICONDUCTORS AND CERAMICS AT ELEVATED TEMPERATURES.

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Load-displacement indentation tests have been performed in single crystals of semiconductors (Ge) and ceramics (fully stabilized cubic zirconia) on a newly designed displacement - sensitive hardness tester capable of performing experiments up to 800 °C. The deformation substructure in the vicinity of the indentation impressions was investigated using selective etching. The energy dissipated during the loading-unloading indentation cycle has been measured and compared with the extent and the structure of the deformation zone. Effect of the indentation loading rate on the deformation structure and the dissipated energy has been investigated. It is shown that the traditional mechanisms of energy dissipation due to cracking, twinning and dislocation plasticity are not sufficient to account for experimental data, and nonequilibrium point defect generation and indentation-induced phase transformation have to be considered.

ROSETTE MICROSTRUCTURE IN INDENTED (001) GA AS SINGLE CRYSTALS AND THE α/β ASYMMETRY

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Room temperature Vickers indentations are performed at room temperature on the (001) face of a n-type GaAs single crystal. The plastic zone around the indents is investigated by Transmission Electron Microscopy (200 kV and 1 MV). Series of 20 x 20 indentations (applied load 0.049 N) are made in a square arrangement with distances of 50 μm in both directions. Samples are thinned from the back side.

The plastic zone consists in:

(i) a highly strained region around the impression which results from the glide of perfect dislocations on converging and diverging planes beneath the indentor

(ii) rosette (perfect) dislocations with Burgers vector parallel to the (001) plane. They look like elongated hairpins; their long arms are screw. Rosette dislocations extending along [110] (respectively [1-10]) have their non screw parts of α (respectively β) type. The α/β asymmetry is not evidenced in our experiments since perpendicular rosette arms have similar lengths.

The hairpin shape of rosette dislocations, as well as the observation that they never emerge at the sample surface, suggest that they are nucleated rather deeply in the crystal, probably on indent facets.

(iii) microtwins which are observed only on {111} planes in zone with the [110] direction (α rosette). They are due to the propagation of identical Shockley partials on adjacent close-packed planes. The shape of the twinning dislocations indicates that they are nucleated on - or very close to - the indented surface as partial dislocation half-loops: by contrast to what is observed for perfect rosette dislocations, twinning dislocations intersect the sample surface.

It has been previously reported that the etch pit pattern around indents in (001) orientated GaAs single crystals exhibits a twofold symmetry, with long and short branches along [110] and [1-10], respectively. This was interpreted as resulting from the intersection of α and β perfect dislocations, respectively, with the surface, leading to the conclusion that the observed pattern is due to the different mobilities of α and β dislocations in this compound. The present results indicate that the observed twofold symmetry in the etch pit pattern should rather be attributed to an anisotropy in twin nucleation and propagation.

The reason why the asymmetry in dislocation velocities is not evidenced in low temperature indentation experiments (similar observations have been reported in other III-V compounds), even though it was clearly evidenced from TEM *in situ* deformation experiments at 350 °C, is not yet clearly understood. Nevertheless, it is suggested that the occurrence of twinning should be taken into account to describe the low temperature mechanical behaviour (hardness anisotropy, asymmetry in the crack extension, ...) of III-V semiconductor compounds.

More generally, it is suggested that great care should be taken in analysing the data obtained from etching experiments.

RECOGNITION AND DISTRIBUTION OF A(g) AND B(g) DISLOCATIONS IN INDENTATION DEFORMATION ZONES ON {111} AND {110} SURFACES OF CdTe

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Indentation-induced plastic microdeformation subdivided into rosette and tetrahedral glide was studied on the low-indexed surfaces of undoped p-CdTe samples by means of SEM-CL employing low temperature and depth-resolved investigations.

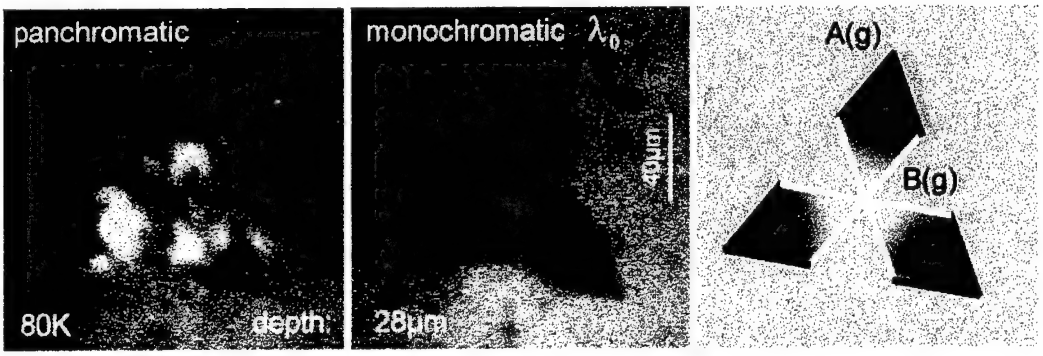
The CL microscopy proved dominating activation of the main $\{111\}\langle 0\bar{1}1\rangle$ slip systems resulting in generation of polar dislocation half-loops made-up of leading 60°-related A(g) and B(g) and trailing screw-type line segments with common Burgers vector $\bar{b} = a/2\langle 0\bar{1}1\rangle$. The defect arrangements could be recognized by utilizing distinct CL contrast properties of A(g) and B(g) dislocations in CdTe.

This work deals with a theoretical and experimental analysis of the distribution of A(g) and B(g) dislocations in the tangential and volume deformation field. The present results show a correlated propagation of A(g) and B(g) dislocations in rosette slip and tetrahedral glide processes, too. The spatial dislocation configurations observed are being related to advanced glide prism models developed for the deformation zone caused by indenting the {111} and {110} sample surfaces, respectively. The experimental findings verify the theoretically expected structure of <110> glide prisms in zincblende crystals as:

$$\{\bar{1}\,\bar{1}\,\bar{1}\}_B\{11\bar{1}\}_B\langle\bar{1}10\rangle\{111\}_A\{\bar{1}\,\bar{1}\,1\}_A .$$

This notation includes the pairs of conjugated $\{111\}_{AA\text{ or }BB}$ glide planes corresponding to the $\langle 1\bar{1}0\rangle$ slip direction.

In accordance with A or B polarity of the glide planes, the internal deformation flow is thought to be realized likewise by A(g)- and B(g)-related half-loops as could be experimentally observed in the rosette as well as tetrahedral glide prisms. The distinct defect arrangements revealed on the {111} and {110} samples yield a self-consistent identification of the crystallographic polarity of the A(g) and B(g) dislocations.



SEM-CL: Verification of tetrahedral glide prisms in (111) sample, corresponding model

THE ORIGIN AND PROPERTIES OF THE NEW EXTENDED DEFECTS IN SI AND SIGE

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The recent investigation of microplastically deformed Si crystals added one more new type of extended microdefects [1]. The defects arise in all Si crystals, are needle-like and have specific morphology. An important fact is that the defects are generated namely by moving dislocation. However, the elements of defects crystallography and its properties were unclear up to now. A particularly interesting question is that of the origin of the defects. In this paper an attempt is made to understand more general peculiarities of the microdefects generation in crystals with diamond lattice. The nucleation, morphology and electrical activity of the defects in Si and SiGe were investigated by photoetching, EBIC and Nomarski microscopy.

It was found that the defects arise as well as in SiGe crystals and have similar elements of crystalography. However, the process of the defects formation is more complicated, A strong dependence on Ge content is revealed. Precise photoetching experiments shown that as a rule the defect axis is < 110> and defects lie near by dislocation slip plane. More complicated defect axis are found. Cross-section experiments have shown that the defects have length up to 50-100 μ. EBIC imaging revealed noticeable contrast in the bands containing arrays of the defects. Qualitatively the electrical activity was confirmed by photoetching experiments.

The origin of the defects is discussed. It is supposed, that the defects are agglomerates of mainly self-interstitials generated by moving dislocation. It is possible that additional gettering effects take place. Very likely that the defects growth is cooperative process and the observed phenomenon is common for material with diamond lattice.

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GETTERING OF Fe AT THE END OF RANGE LOOPS AND TWIN BAND INTERFACES IN Fe-IMPLANTED InP.

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A study of the influence of extended defects on the Fe distribution in Fe-implanted InP is presented.

Extrinsic end of range (EOR) dislocation loops were always produced upon annealing of InP implanted with Fe at various energies (0.2-2 MeV) at doses above the amorphization threshold. The majority of the EOR loops were of the 1/3<111> Frank type. The other ones were perfect with 1/2<110> Burgers vector. The EOR loops have undergone loop coarsening as they increased their size by increasing the annealing time, very likely by a mechanism of interstitials transfer from the smallest to the largest loops. For implants at the highest energies (2 MeV) twin bands have additionally formed due to the greater damage associated with such high energy, that could not be annealed out completely. The twin bands terminated with a tangled network of dislocations.

An anomalous diffusion of the implanted Fe has also taken place upon annealing as Fe accumulation peaks occurred at specific depth positions, i.e. at the positions of the EOR dislocation loops as well as of the bottom interface between the twins bands and the fully recovered sample. The Fe anomalous accumulation increased with increasing annealing temperatures and time.

The above results indicate that the anomalous diffusion of Fe is determined by its trapping at the EOR loops and bottom interfaces of the twin bands, rather than by formation of Fe-P complexes as suggested in the literature. Such trapping should occur by Fe gettering by the partial dislocations bordering the EOR loops and by the strain fields associated with the tangled dislocations at the bottom interface of the twin bands. Very likely the anomalous Fe distribution is also affected by the enhanced diffusivity of Fe in the EOR loops region. The formation of the EOR loops and the continuous exchange of interstitials among them during the coarsening process is expected, in fact, to help to maintain a supersaturation of (In) self-interstitials in this region that may enhance the Fe diffusion.

SELECTIVE ELECTROCHEMICAL PROFILING OF THREADING DEFECTS IN MISMATCHED InGaAs/GaAs HETEROEPITAXIAL SYSTEMS

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We report on the study of the defect structure in MBE-grown (100) InGaAs/GaAs mismatched heteroepitaxial systems by selective electrochemical (anodic) etching [1]. The In content and layer thicknesses are varied between 0.03-0.3 and 0.02-5 μm respectively (the thicknesses are typically above critical layer thickness). The growth was controlled by RHEED intensity oscillation to achieve good layer quality and to determine the composition [2]. Different aqueous electrolytes and bias voltages were tried to optimise the etching conditions. HCl-based solutions were found appropriate for the development of crystal defects both in InGaAs and in GaAs. The etched surfaces are studied by scanning electron microscopy and optical microscopy. By incremental layer removal, we mapped the depth profile of the dislocation density. The density of defects is found to depend on layer thickness and composition. In the thickness and composition range we studied, the defect density is inversely proportional to the layer thickness and increases with In content. The results are compared to various theoretical models of threading dislocation annihilation [3]. The defect distribution in the substrate was studied as well, and the lateral defect distribution in the layer is correlated with that of the substrates. In certain cases, a cross-hatch pattern is observed; its occurrence is correlated with growth mode and the observed defect behaviour.

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MAKYOH TOPOGRAPHY FOR THE STUDY OF LARGE-AREA EXTENDED DEFECTS IN SEMICONDUCTORS

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Makyoh topography is a simple but powerful method for the study of macroscopic surface defects in semiconductor wafers and layer structures. The principle of the method is simple: any irregularity of the sample surface acts as (local) concave or convex mirror therefore a collimated light beam impinging on the surface produces an image on a screen that somehow reflects the sample morphology. The method is extremely sensitive and is able to detect e. g. dislocation slip lines, subsurface defects, process-induced defects and local stresses. Despite of the simple principle, the mechanism of the image formation and the relation of the morphology and the image contrast have remained unclear, which clearly hinders its application. This contribution aims a more quantitative approach to the understanding of the Makyoh image formation mechanism. First, some general relations are given on the optical settings. Then, optical ray-tracing simulations of an isolated defect (hillock or depression) and a periodic (sinusoidal) surface are presented for different optical settings. Optimum working conditions are established, and some general features of the imaging are pointed out. Some supporting experimental images from GaAs-based epitaxial structures and wafers are shown as well.

This work was supported, in part, by the (Hungarian) National Scientific Research Fund (OTKA) through Grant F 25224.

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MAKYOH TOPOGRAPHY: DIRECT OBSERVATION OF THE DEFECT DISTRIBUTION IN MBE GROWN LAYERS

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The magic - mirror, or Makhyoh, topography technique is applied to study the defect distribution in molecular beam epitaxially grown layers (MBE). In order to facilitate the visualisation of the defects in the epitaxial layers, the used [100] GaAs substrates are treated by a "developing" polishing procedure (0.5 μm Al_2O_3 abrasive on cloth for 15 minutes at a speed 0.1 m/s under pressure of 50 kN/m^2 .

It is argued that the surface relief of the substrate generated through the "developing" treatment is reproduced by the surface of the MBE grown layers and can be observed in the magic mirror images. The image pattern is generated by the reproduced substrate relief and because the majority of defects in epitaxial layers is generated by imperfections of the substrates, it reflects the defect distribution in the MBE grown epitaxial layers.

It is also shown that standard substrate preparation processes often leave subsurface stressed areas, the presence of which has to be taken into consideration in the MBE technology.

DEFECTS AND A RADIATION-ENCHANCED DEFECT PROPOGATION IN ZnSe /(001) GaAs MBE BUFFER LAYERS

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Since the first blue-green electron-beam pumped lasers had been realized in heterostructures of ZnSe/ZnCdSe with lifetime about few hours at 300K [1], their degradation was shown to be determined by the quality of the ZnSe buffer layer, which produced dislocations sprouting in the active layer. In this work point defect-dislocation interactions in ZnSe/(001)GaAs buffer layers grown by MBE was investigated.

The influence of growth condition variations and epilayer thickness on strains and depth dislocation distribution in ZnSe buffer layers were studied. To investigate the degradation mechanism, the influence of low energy electron irradiation (E=18 keV, I_e=14 A/cm^2 in scanning regime) and UV-irradiation which result in the same degradation processes as carrier injection as well as thinning of the substrate on epilayer properties were examined. We used high-energy electron and X-ray diffraction methods combined with exciton and impurity photoluminescence spectroscopy as well as Hall-, conductivity and photoconductivity measurements for control of growth and properties. Special attention was paid for depth and lateral non-uniformity investigations. The influence of epilayer thickness and growth conditions on dislocation distribution was studied. The interdiffusion of Ga and Zn through interface during growth as well as radiation enhanced defect transformation which depend on dislocation distribution were observed.

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ANISOTROPIC RELAXATION OF THIN LAYERS WITH ZINCBLENDE STRUCTURE

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Recently, due to development of new technologies such as MBE and MOCVD, the studies of thin layers have been carried out very extensively. Usually crystallographic data are explained assuming the tetragonal distortion of the unit cell. In our report the directional character of in plane strain is presented.

The investigated layers of MnMgTe/GaAs, CdTe/GaAs, AlGaAs/GaAs, GaInP/GaAs were of 1-10 μm thicknesses. The structure of samples was examined using high-resolution X-ray diffractometry. The application of a four-reflection Bartels monochromator and of a two-reflection analyser ensured measurements of the lattice parameters with ppm accuracy. Moreover, our experimental set-up allowed us to examine the samples by the reciprocal lattice mapping technique. The X-ray topographs were obtained using a double-crystal diffractometer set in a non-dispersive mode. Measurements were made with the sample aligned with either [110] or [-110] direction perpendicular to the diffraction plane. From our experiment it follows that for majority of investigated samples lateral strains are anisotropic. It means that unit cell of layers is not tetragonal but posses a lower symmetry. Our results indicated that in layers with the zincblende structure the directional relaxation took place. This effect can be explained by higher mobility of [-110] oriented dislocations in comparison to those oriented in the [110] direction. Therefore, the different dislocation density in the both directions can be expected leading to the observed anisotropy of lattice misfit relaxation. Our results are in agreement with those reported by Tanner *et al.* for AlAs/GaAs layers [1] and Heinke *at.al.* for CdTe/CdTe[2].

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THE HRXRD DETERMINATION OF THE SHAPE OF INTERFACES IN THE LATERALLY INHOMOGENEOUS A_3B_5 SUPERLATTICES

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The method of the X-ray diffractometric investigation of the shape of the interface between two adjacent crystalline layers in InGaAs/InP superlattices that have intentionally introduced lateral gradient of chemical composition is presented. The method consists in finding the distribution of elements in the superlattice crystal, for which the best fit between calculated and experimental diffraction pattern is achieved. The calculation of the diffraction pattern was performed by means of the computer program based on the kinematical theory of X-ray diffraction. This program is not limited by the shape of the chemical composition modulation wave, so that any change of the composition even concerning only one atomic plane could be taken into account. The X-ray diffraction profile obtained for superlattice crystals with lateral gradient of chemical composition shows up characteristic broadening of satellite reflections, so that the distribution of elements in the growth direction results from satellite intensities, and the lateral distribution may be obtained from the profile broadening.

NON CONVENTIONAL RECIPROCAL SPACE INVESTIGATION TECHNIQUE APPLIED FOR $A_{II}B_{VI}$ SUPERLATTICES

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We present an X-ray diffractometric study of 150-period CdTe/ZnTe superlattice grown on (001) GaAs substrate misoriented with an offcut angle of about 2°. In this case the direction of the tilt angle between (001) planes of the superlattice is not coplanar with the surface normal and the (100) GaAs direction. Our goal was to work out a method of investigating such case based on performing one-dimensional scan of the reciprocal space that passes through the gravity centre of each satellite reflection. This is achieved by setting up the crystal so that the vectors normal to reflecting planes of the substrate and superlattice lie simultaneously in diffraction plane and then performing series of alternating (θ/2θ) and (ω) scans covering the whole required scanning range. To this end it is necessary to establish the co-ordinates in reciprocal space of initial and final points of the line, along which the scan should be performed and then apply the Bresenham algorithm (designed first to plot a strait line on a raster device) to find the range of each (θ/2θ) and (ω) scan. Such experimental method assures that the intensity of each satellite reflection, modulation wavelength, tilt and misorientation angles will be properly measured. The values of the tilt angle β and the wavelength of the modulation wave Λ can be calculated applying the estimated centre of gravity coordinates of the nodal and satellite reflections to the following formulas:

$$\beta = \frac{1}{2m+1}\sum_{i=-m}^{m}\omega_i$$

$$\Lambda = \frac{1}{m}\sum_{i=1}^{m}\frac{\lambda|i|}{\sqrt{\sin^2\theta_i + \sin^2\theta_{-i} - 2\sin\theta_i\sin\theta_{-i}\cos(2\beta)}}$$

Where i stands for the satellite number and m is the total number of satellites taken into account. This procedure applied to the investigated CdTe/ZnTe crystal determined: the modulation wavelength Λ = 7.0181nm [1], the tilt angle β = -0.00143° and misorientation angle ε = 1.8°. Because the tilt angle β and the misorientation angle ε are related to the relative lattice mismatch Δd/d by the equation [2]:

$$\tan(\beta) = (\Delta d/d)\tan(\varepsilon)$$

hence it follows that Δd/d = 0.00079.

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High Resolution XRD and Reflectivity Studies of Epi-Ready Substrate Surfaces.

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Neodymium Gallium Perovskite single crystals are used as substrates for high temperature superconductor epitaxial layers and are the ones of the most promising substrate materials for epitaxial growth of GaN. Besides of the structure matching, good quality epi-layers can be grown only on the crystallographically perfect substrates with well-prepared smooth and damage free surfaces.

Triple crystal X-ray diffractometry have been used to determine defects in $NdGaO_3$ epi-ready wafers. The high resolution measurements were realized by taking curves at ω mode (ω = var, 2θ = cons). By reciprocal space mapping, a distribution of the scattered intensity near reciprocal lattice points was found, which is characteristic for mechanical treatment of wafer surface. The two dimensional X-ray diffraction measurements were performed after the mechanical polishing as well as after the etching procedure.

Additionally, the results of the X-ray reflectometry investigations of the surface perfection after the mechanochemical treatment are presented.

STUDY OF EXTENDED DEFECTS STRUCTURE INDUCED BY PULSED LASER ANNEALING IN IMPLANTED SILICON CRYSTALS

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It was observed previously [1] that the dislocation structure was created in the Si (111) wafer implanted with Ge ions of the energy 80 keV and dose of $5x10^{15}$ ions·cm^{-2} as a result of an annealing by means of a pulsed excimer laser beam when the energy density of laser radiation was high enough. To obtain an information about melting dynamics induced in material by excimer laser radiation the theoretical calculations based on the Fourier equation of the heat flow were performed. The threshold values for surface melting [2] and the optimal values of the radiation energy density causing a full melting of amorphous layer aa well as a start of recrystallization process [3] were determined.

Supposing that dislocation structure was formed in the surface layer for laser energy density higher than the optimal value, we carried out experimental investigations of several Si crystals. The crystals were first implanted with different ions with energy and dose causing amorphization of the surface layer. Then they were annealed by using a pulsed excimer laser radiation of different energy densities, lower and higher than the threshold value calculated previously. The samples were studied using a number of methods, namely, X-ray topography, RHEED and Nomarski microscopy.

According to our expectations, we have observed the dislocation networks created in implanted and annealed Si crystals when the optimal energy density of the laser radiation was exceeded.

This study was partly supported by the Committee for Scientific Research under the grant No. 113/PO3/95/09.

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DISLOCATIONS GENERATED in Cz Si ANNEALED UNDER NORMAL or HIGH PRESSURE

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Dislocations generated during annealing in as-grown dislocation – free Cz Si were investigated by X-ray topography.

The dislocation arrays with Burgers vectors parallel to the crystal surface and oxygen precipitates were observed in crystals annealed at normal pressure in two-step and three-step annealing processes. The set of dislocations beginning from the crystal edge was observed in the crystal (111) oriented, annealed at 750°C(4h) , 1050°C (1h) and 1150°C(4h) (Fig.1).

In the crystal ((001) oriented) annealed at 900°C (1h) and 1150°C (10h) – three sets of dislocations (straight and in the form of half-loops anchored at silicon oxide precipitates, Fig.2,3) were recognized in all crystal volume.

Besides of many oxygen precipitates, two arrays of dislocations of half-loop shape with Burgers vectors parallel to the crystal surface were observed in the crystal ((111) oriented) annealed at 750°C (1h) under 6 kbar hydrostatic pressure (Fig.4). The dislocations were punched out from the surface of large misfitting region of crystal (situated near the crystal edge) acting as shear-stress centre (according to the Ashby and Johnson model).

Fig.1

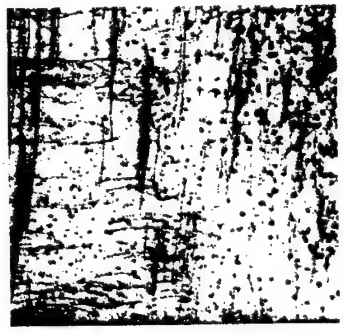

Fig.2

Fig.3

Fig.4

EFFECT OF STRESS ON CREATION OF DEFECTS IN ANNEALED CZOCHRALSKI GROWN SILICON

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Oxygen admixture always present in Czochralski grown silicon, Cz-Si (representing in fact the supersaturated solid solution of oxygen in silicon) undergoes transformations at higher temperatures, which can result in creation of different oxygen - related defects. Understanding the reason of stress effect on such transformations is of interest also for practical applications (Cz-Si is still the most important semiconductor for microelectronics).

The previously reported [1] information on effect of hydrostatic pressure at annealing of Cz-Si is updated and recently published data, e.g. [2 - 4], are reviewed in this work.

Cz-Si samples with oxygen interstitials, O_i, concentration up to above $10^{18}cm^{-3}$ (sometimes preannealed at 10^5Pa to create different oxygen - related defects) as well as the samples of silicon implanted by oxygen were subjected to pressure treatment at up to 9GPa in diamond anvil cell, DAC, or annealed at up to 1620K at argon (helium) pressure up to 1.6GPa for up to 20h (treatments at about 720K) or for up to 0.5h (treatments at the highest temperatures). After HP treatment the sample properties (defect structure) were determined by electron microscopy, Fourier Transform Infrared Spectroscopy, photoluminescence, PL, selective chemical etching, ellipsometry, X-ray (synchrotron) topography, and reciprocal lattice mapping, DLTS as well as by other methods. In dependence on hydrostatic pressure, HP, value and on treatment temperature and time, it were observed different HP - induced effects:

- DAC treatment at 300K of the samples with previously created oxygen - related defects resulted in massive creation of dislocations;
- HP - anneal at $\leq$ 1000K caused considerable enhancement of the rate of thermal donors creation with (HP - related) PL at about 0.78eV;
- HP - anneal at 1170 - 1420K of the samples with before - created nucleation centres can result in massive oxygen precipitation with strongly HP - dependent enhanced concentration of dislocations and of stacking faults, as it followed from increased intensity of the D1 and D2 PL lines;
- HP - anneal at >1280K of the samples with before - created oxygen precipitates resulted in retarded dissolution of oxygen - related defects in the silicon matrix.

HP during annealing of the samples resulted typically in creation of higher concentration of smaller defects (in comparison to the case of annealing at 10^5Pa) with enhanced percentage of oxygen interstitials removed from the Si lattice .

At least part of above - listed observations can be explained in terms of HP effect on oxygen diffusivity and on misfit at the oxygen defect / silicon matrix boundary.

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STRUCTURE OF OXYGEN AND SILICON INTERSTITIALS

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Internal extended defects in crystals, such as dislocations, are creating regions of compression and strain. The electronic and geometrical structure, kinetic properties (diffusion rate) of interstitials and other point defects are changing in the regions of compression and strain. The defect geometry and electronic structure were studied, using the model of molecular cluster.

Ab initio quantum chemical simulation of oxygen and silicon interstitials O_i and Si_i in silicon was performed. The reference ideal crystal was represented by a molecular cluster consisting of 17 (for O_i) or 13 (for Si_i) Si atoms, with H pseudoatoms at dangling bonds. This model could serve to investigate pressure effects at internal interfaces created during O precipitation in Cz-Si. Pressure was simulated by putting a smaller value for the lattice constant. O_i defect was shown to be linked with two Si atoms standing a bit apart from the middle of Si-Si bond. Si_i defect is linked with three Si atoms standing in the middle of the longest side of Si-Si-Si triangle. The distance of the Si interstitial from two side atoms is 0.219 nm, from the middle atom - 0.246 nm. In both cases, the nearest neighbours of the interstitial are shifted from their positions in ideal lattice outside by approximately 0.05 nm.

Under a uniform compression causing 0.25, 0.37, or 5.0 per cent reduction of the lattice constant, the angle O-Si-Si in O_i defect equilibrium state grows from 30 to 40 degrees, and in diffusion transition states O atom moves away from the nearest Si atom, but the Si atom approaches its position in the ideal lattice. The general tendency for higher pressure seems to be lower influence of chemical bonding and more efficient use of free volume during the O transition. The migration activation energy for O_i defect was estimated as 2.73 eV at the atmospheric pressure, and 2.70, 2.68, and 1.92 eV for the lattice compressed by 0.25, 0.37, or 5.0 per cent, respectively.

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INFLUENCE OF DISLOCATIONS ON NITROGEN-OXYGEN COMPLEX IN SILICON

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Nitrogen in silicon can suppress the formation of microdefects and increase the mechanical strength. It is important that the nitrogen-doped silicon can improve the quality of silicon material and decrease the thickness of the silicon slices, which are large in diameter. While nitrogen is induced into Czochralski silicon (CZ) crystal during the growth process, nitrogen-oxygen (N-O) complexes are formed. In this paper, we have investigated the influence of dislocations in nitrogen doped CZ silicon on N-O complexes. Samples were come from a nitrogen doped CZ silicon crystal that was grown under a nitrogen atmosphere. The samples were divided into two groups. The dislocation was induced in the one of the groups. The density of the dislocations was $5*10^4$ cm^{-2}. Both of the two groups were annealed at 650℃ for different times. It was found that N-O complexes were formed after annealing for 10 min. The intensity of N-O complexes increased with the annealing time. Two hours late the intensity of N-O complexes reaches a maximum in dislocation-free sample, and then decreases with the annealing time. After annealing for 60 hours, the N-O complexes were eliminated. However, the intensity of the N-O complexes in the sample with dislocation decreases with the annealing time after annealing only for 30 min. Three hours late all of the N-O complexes were annihilated. This indicates that the dislocations suppress the formation of the N-O complexes. It is considered that nitrogen and oxygen diffuses fast into dislocations respectively and locks the movement of the dislocations. The mechanism that dislocations suppress the formation of N-O complexes is also discussed in detail in this paper.

ON THE INFLUENCE OF DISLOCATIONS ON THE LUMINESCENCE OF Si:Er

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The observation of an optical activity in Er-doped silicon has set off a great interest since the luminescence emission peak occurs at 0.806eV, a wavelength corresponding to the absorption minimum of optical fibers used in communication devices.

The luminescence is influenced by the presence of defects whose nature and properties are still largely unknown and, moreover, it has been observed that the interaction of Er with other impurities such as oxygen enhances the material optical activity.

We have studied by optical and electrical methods the properties of the defects which take part in the radiative process to possibly identify which ones affect the luminescence of the material. Er can be introduced by different methods in the Si matrix (ion implantation, MBE, diffusion etc.) and each one produces quite different behaviors. We have characterized for the first time Er-doped Si samples grown by the Liquid Phase Epitaxy (LPE) method, a relatively simple and inexpensive technique, by means of photoluminescence (PL), cathodoluminescence and deep level transient spectroscopy.

PL measurements have shown the presence of two emission bands which coincide with the lines labeled D1 and D2, observed in silicon in the past and attributed to the presence of dislocations. Since line D1 fortuitously coincides within a few meV with the energy of the transition $^4I_{15/2} \rightarrow {}^4I_{13/2}$ of Er^{3+}, it could at least partially cover the Er-related emission. Furthermore, as Er and O are gettered at dislocations, the dislocation optical activity might be influenced by their presence and play a significant role in the material overall luminescence.

A thorough investigation of these samples, therefore, allows to get a better insight into the impurity assisted radiative recombination at dislocations, which has to be taken into account when characterizing Er-doped LPE silicon.

Cu_3Si-Precipitates in Silicon: An Example for Deep Bandlike Defect States

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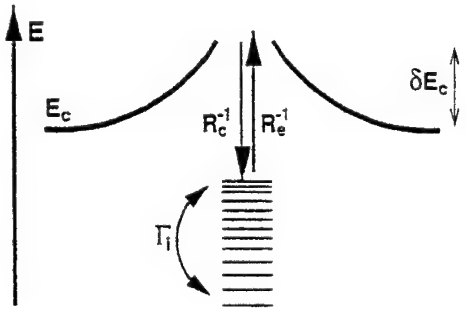
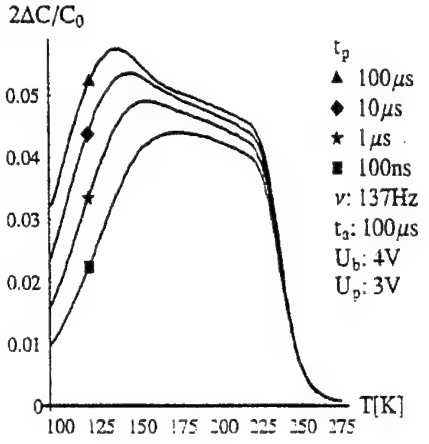
Deep level transient spectroscopy (DLTS) of Cu_3Si-platelets in silicon formed by rapid quenching from diffusion temperature show a surprisingly broad line shape. The electronic properties of this extended defects are explained by assuming a band of deep defect states in the band gap, its occupation being given by quasi Fermi distribution. Recent annealing experiments indicate, that the defect density of states is twodimensional.



bandlike: $\Gamma_i \ll R_e^{-1}, R_c^{-1}$



This model of bandlike states implies that the thermal electron emission practically stems from all states above the quasi-Fermi level. We show that this leads to a logarithmic dependence of the transients on time and to the property of 'confluent transients', i. e. transients with different initial occupations become indistinguishable after a certain time t_1. The time t_1 decreases exponentially with rising temperature. This property also serves for the explanation of the fact that the high-temperature sides of DLT spectra with different pulse length coincide.

We demonstrate by simulations that the shape of the DLT spectra can be explained by assuming a high occupation of the defect in its neutral state. As a consequence the defect is mainly positively charged during the DLTS experiment and offers an attractive potential to electrons. Thereby the electron capture namely in the Debye tail is enhanced, which serves for the characteristic features of the spectra.

EFFECT OF DEFECT BANDS ON THE ELECTRICAL CHARACTERISTICS OF IRRADIATED GaAs AND Si

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Electrical characteristics of bombarded GaAs and Si wafers have been studied. The n-GaAs wafers with a free electron concentration of about $2x10^{17}$ cm^{-3} were irradiated by 1 MeV neutrons with different doses in the range of $1x10^{12}$-$1x10^{16}$ cm^{-2}. Au Schottky contacts were prepared to the irradiated wafers. The effect of the bombardment was studied by DLTS technique and by current-voltage (I-V) and capacitance-voltage (C-V) measurements in the temperature range of 100-360 K. It has been observed that for low irradiation doses ($1x10^{12}$-$1x10^{13}$ cm^{-2}) only the EL2 trap appeared in the DLTS spectra. The concentration of this trap was found to increase with the dose up to $1x10^{14}$ cm^{-2}. Higher irradiation doses gradually decreased the EL2 density, and created a broad DLTS peak centred at about 180 K, which has been attributed to the "U band", indicating the presence of defect complexes in Si. The amplitude of this peak increased with the dose of irradiation. The I-V and C-V measurements suggested that the Fermi-level pinning position moved towards the conduction band edge with the increase of the irradiation dose.

The p-Si wafers with a doping level of about $2x10^{15}$ cm^{-3} were irradiated by protons with an energy of 650 eV by using plasma immersion implantation technique. The hydrogen introduced into the reactor chamber contained 1% PH_3. The duration of the bombardment was 20 and 40 min. After the bombardment a part of the wafers have got a two step annealing process in forming gas at 600 °C for 10 min and 900 °C for 5 min. Al Schottky contacts were prepared to the bombarded wafers. The wafers were studied by the same methods as described above. DLTS measurements have shown that the unannealed wafers also exhibited a broad DLTS peak centred at about 260 K, which has also been attributed to a defect band, indicating the presence of extended defects. In the annealed wafers no defect band was observed, but three peaks were obtained that can be connected with Fe-B, Cr-B pairs and Mo impurity. The concentrations of these impurities was higher for the wafer bombarded during 40 min by about one order of magnitude, than those for the wafer bombarded during 20 min. The I-V and C-V characteristics depended also strongly on the bombardment and annealing process.

In this paper the similarities and differences of the electrical characteristics obtained on the neutron bombarded GaAs and proton bombarded Si wafers will be discussed.

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OXYGEN EFFECT ON DISLOCATION ELECTRICAL AND OPTICAL PROPERTIES

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Dislocations in Cz p-type Si oxygen-rich (>10^{18}cm^{-3}) single crystals have been investigated by deep level transient spectroscopy (DLTS), and by photoluminescence (PL) techniques. They were introduced either by four point bending or by elastic bending at room temperature in a cantilever mode and subsequent heating (625-700°C) under stress in a pure argon atmosphere. The deformation duration was changed from 15 minutes to 4 hours. It has been observed that the intensity of the PL dislocation related spectrum consisting of four well known D1-D4 lines decreases with an increase of deformation duration. A subsequent transition metal contamination annealing does not lead to a restoration of these PL lines quenched under prolonged deformation.

Dislocation related DLTS spectra in such crystals were also found to depend on a deformation duration, decreasing in intensity when increasing deformation time. The decay of DLTS signal with time, similar to that of PL decay, was found to depend on oxygen and/or other impurity contents. In some crystals, no DLTS spectrum was revealed even after 15 minutes of deformation at 625°C. Similar to the PL, if the DLTS spectrum is not observed after a long deformation, it can not be restored by a subsequent transition metal contamination annealing. Preliminary investigations have shown that the main parameter responsible for the DLTS signal quenching seems to be the dislocation pathway, that is the way covered by dislocations during their motion through the crystal under stress, but not the deformation duration itself.

To explain the observed quenching of PL and DLTS dislocation related spectra with an increase of deformation duration in Si crystals with a high oxygen content, electron beam induced current (EBIC) measurements were carried out on such samples which showed a pronounced contrast at dislocations. Besides a strong compensation of shallow acceptors was observed after the deformation. Therefore, the decay of the PL an DLTS signals can not be explained by a decrease of dislocation electrically active center concentration due to an increase of deformation duration. Instead, it seems that in crystals with a high oxygen content the concentration of dislocation related centers increases compared to FZ Si samples or to Cz ones with a lower oxygen content. Thus, the results obtained could be explained under the assumption that dislocations gather oxygen during their motion and therefore the oxygen concentration in dislocation cores depends both on the oxygen bulk concentration and on the dislocation pathway. If the concentration of dislocation related centers increases with the oxygen concentration in the dislocation core, this could quench the PL signal due to the increase of recombination velocity. The DLTS signal decay could be explained by the formation of electrostatic barrier near the dislocation which might prevent the filling of dislocation related defects. Actually, if this barrier is high enough and remains in the depletion region, the centers located near the dislocation core can not be filled which leads to a decrease of the DLTS signal.

TRANSFORMATION OF ELECTRICAL ACTIVITY OF EXTENDED DEFECTS IN SILICON POLYCRYSTALS UNDER ANNEALING AND HYDROGEN PLASMA TREATMENT

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Grain boundaries (GBs) and dislocations are the main types of extended defects (EDs) that control electrical parameters of devices manufactured on the base of polycrystalline silicon. So the development of different methods of EDs electrical activity suppression is important task for the present-day silicon material science.

In this work influence of different types of heat treatment and hydrogen passivation on electrical activity of EDs in EFG ribbon silicon is studied. Samples with special, deviated (nearly-coincident) and general (random) GBs were heat treated in vacuum, oxygen, air and also in O_2-HCl mixtures at 1000-1200 °C. Besides, influence of cooling rate (1, 16, 500 °C/min) after heat treatment was investigated. Hydrogenation of samples was carried out in a Kaufman source, in a reactive ion etching system (RIE) with hydrogen plasma and in a system with low energy (10 eV) atomized hydrogen flow (LEAH) produced by HF-decomposition of molecular hydrogen.

Electrical activity of EDs in as-grown and annealed samples was tested by EBIC and LBIC measurements and temperature dependencies of resistivity and Hall effect. Besides, activity of individual GBs was also estimated by transversal I-V and C-V characteristics (when current was normal to GB plane) and spreading resistance measurements.

Our experiments have shown that high temperature annealing resulted in full moderation of electrical activity of dislocations and their piles-up and sharp decrease of activity for weakly deviated from special orientations $\Sigma 3$ grain boundaries. By contrast, random GBs raised their activity under heat treatment. Among GBs studied, the lowest activity was characteristic of GBs in samples cooled with a moderate velocity (16°C/min) after annealing. At the same time, superlow (1°C/min) and superhigh (quenching) cooling resulted in increasing of GB electrical activity (intergrain barrier increased).

Our investigations have exhibited a number of distinctions in the character of GB hydrogen passivation for random and deviated GBs in as-grown and annealed samples. Under implantation of H_2^+ in a Kaufman source (1.7 KeV; T = 350°C; j = 1.5 mA/cm^2; 2-15min) activity of near-coincedent $\Sigma 3$ GBs disappeared completely, whereas for random GBs it decreased only partially. Hydrogenation in RIE and LEAH plasma of as-grown samples had an twofold impact on electrical properties of GBs in silicon ribbons. Under increase of exposure time in the range 0 -120 min, electrical properties of grain-bulk did not changed although activity of the both types of GBs decreased. For exposure times higher than 120 min, decreasing of GB activity was accomponied by generation of point defects and lowering of carrier mobility in the grain-bulk. For annealed samples random GBs activity (that has been grown during heat treatment) decreased nearly to zero after hydrogen plasma treatment, whereas deviated GBs passivated more slowly (as in as-grown samples). Besides, in annealed ribbons point defects in the grain bulk did not generated during plasma hydrogenation.

ELECTRON-HOLE DROPS ON DISLOCATIONS IN SILICON

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The processes of electron-hole drops (EHDs) formation and their migration in a crystal, containing a significant number of dislocations, can have the features as compared with dislocation-free crystal. In the present report the results of photoluminescence study of the EHDs in silicon at 4.2 K are presented. Dislocations in samples studied were generated by plastic deformation at 680 °C. It has been shown that:

1. Dislocations in silicon are centers of the EHDs condensation. The threshold of concentration of exitons needed for EHDs formation is decreased when dislocation density (N_D) increasing. Minimum of threshold corresponds to $N_D = 5 \cdot 10^3 - 1 \cdot 10^4$ cm^{-2}. The further elevation of N_D leads to decrease of exciton life time and, as the consequence, to decrease of the excitation intensity.

2. In addition to the line with maximum 1.082 eV in radiation spectrum of the EHDs dislocational silicon contains the line with maximum 1.078 eV. The additional component of spectrum is due to appearance of the specific non-spheroidal EHDs spreading along the dislocation axis. It has been calculated that the line shift is connected with the dislocation fields of elastic stresses. It has been also shown that the radius of cylindrical dislocational EHDs can not exceed 1-2 mm. Spheroidal drops are more probable at greater radii.

3. The existence of dislocation cylindrical EHDs is confirmed also by different character of the dependence of the EHDs recombination radiation intensity on excitation intensity. In a case of dislocation-free samples this dependence is close to cubic, while this dependence is practically squared-like in dislocation silicon.

4. The radiation of the EHDs in dislocational samples is polarized. The polarization degree depends on conditions of plastic deformation of samples. The radiation polarization of the EHDs and dislocation luminescence was not found in the samples with grown-in dislocations.

On the base of these results a model of recombinational statistics for silicon at low temperatures taking into account the presence of a number of recombinational processes (free exitons, exitons on impurities and dislocations, EHDs) is developed. Processes of formation and transformations of EHDs (including dislocational) are described in the frmawork of this model.

TEMPERATURE EFFECT ON INTERFACIAL STATE DENSITY IN THE MOS STRUCTURE

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Abstract :

The main objective in this work is the characterization of oxide semiconductor interface and the modelization of the state density evolution with temperature.
After elaboration of $Al/SiO_2/Si$ structure, the characteristic C (V_G) versus temperature was established with a bench of measurement C-V functioning at the frequency 1MHz. The used silicon substrate of [111] crystallographic orientation present a resistivity in the range 0.2 to 0.5 Ω.cm. The temperature range used during the electric characteristic vary from 25°C to 320°C. At room temperature, the test sample has a flat band voltage which is equal to –2.7 V, this explains the presence of quantity of charges (Q_T) on the oxide/semiconductor interface which is estimated to 7.2×10^{11} charges/cm^2 .
The energetic distribution of the interface states at this temperature is quite flat around the middle of the bandgap.
We note no variation in characteristic C (V_G) for a accumulation and depletion regions, using modelization and electrical characterization. Therefore, in an inversion regions the structure capacitance increases.
Note that we have no change concerning the flat band voltage V_{BP} when the temperature vary from 25°C to 200°C; consequently, the quantity of charges Q_{SS} present in the oxide/semiconductor interface remain constant in this temperature range. Thus, for temperatures greater than 200°C, the characteristic C (V_G) is modified. This modification is induced by the thermal activation resulting from the temperature increase which facilitate the inter-band exchange mechanisms. The charge in the inversion layer due to the minority is increased and the maximal extension of the depletion zone is decreased. When the temperature increases (T>200°C), the interface states density increases, the energetic distribution is modified except in the middle of the bandgap. Indeed, our calculations show clearly that a temperature being about on substrate induce an augmentation of states in the tail of conduction bands. This physical change affect particularly the defects related to dislocations. Therefore, the deep states corresponding to hanging bonds are not affected by the temperature.

Spectroscopic analysis and electrical study of Au/InSb/InP systems.

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Abstract

The great development of the microelectronics and the communication technologies led the world of the researchers to the study of III-V semiconductor made compounds, such as the Indium Phosphide InP. In fact, this kind of semiconductor is utilised making of 1.3 μm to 1.6 μm wavelength laser diodes and also in the Fast Field Effect Transistors design.

In order to realise electronic components of the Metal-Semiconductor type on InP(100), it appears to be essential to know as well the InP-Metal interface properties. The improvement of the physical and electrical properties of such structures needs their annealing in the 300 °C to 400 °C temperature range, well the V element of the semiconductor is very volatile. This fact led to a radical change of the superficial zone of the substrate.

In this work, we are studying, both the restructuration and annealing effects on the electrical parameters of a Au/InP Schottky diode, where its surface is restructurated with a some monolayers InSb film.

For this purpose, we measure the current-voltage characteristics before and after restructuration. We propose, then the study the electrical quality of the elaborated components after the Au/InP interfaces creation without annealing and then after annealing for several heating temperatures (from 300 °C to 500 °C).

The analysis of the measured I(V) characteristics for the Au/InP and Au/InSb/InP samples allow to determine the variations of the electrical parameters. The saturation current Is, the serial resistance Rs, the mean ideality factor n and also the barrier height ϕbn, are respectively equal to 2.10 10-4 A, 19 , 1.8 and to 0.406 V for the Au/InP sample and to 1.34 10-7 A, 300 , 1.78 and to 0.592 V for the Au/InSb/InP sample in the 500 °C annealing case.

This work permits, thus, the evolution study of these electrical parameters related to the restructuration conditions.

INFLUENCE OF DISLOCATIONS ON ELECTRICAL PROPERTIES OF N-TYPE 6H-SiC CRYSTALS

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We have initiated a comparative study in the electrical properties of as-received SiC single crystals with dislocated crystals by performing capacitance-voltage (*C-V*), current-voltage (*I-V*), and thermally-stimulated capacitance (TSCap) measurements. Fresh dislocations were introduced by scratching a {0001} surface (Si-face or C-face) along a $<1\bar{1}20>$ direction using a diamond scriber followed by an annealing (1000°C, 3h). Dislocations were also subsequently characterized using conventional Transmission Electron Microscopy (TEM) and the technique of Large Angle Convergent Beam Electron Diffraction (LACBED). In this paper we compare the results obtained after the deformation step on the (0001)Si face and $(000\bar{1})$C face of n-type commercially 6H-SiC. Whatever the deformed surfaces may be, the deformation step results in strong compensation effects. In both cases, it was found that the as-introduced deep traps are mainly located in the upper third of the bandgap which also promote a significant increase in the series resistance of the diodes. The main difference observed in between lies in the number of trapped carriers. Indeed, a larger compensation effet is observed after deforming the C-face. By TEM, we have shown that the scratching on the (0001)Si face introduces predominantly 30° partials and their core nature was determined to be Si(g). As already observed in 3C-SiC and 4H-SiC, the Si(g) partial dislocations show a smooth morphology whereas the C(g) partials have a zigzagged morphology. However, due to the large carriers trapping the compensation effects observed after deformation are presumed to be caused not only by Si(g) dislocations but also by the other defects generated during the deformation step. When deforming the C-face conventional TEM shows that near the scratches the deformation introduced predominantly zigzagged 90° and 30° partials in the same ratio approximatively whereas only smooth dislocations in shape are obverved beyond. The nature of as-introduced dislocations on this latter face is currently investigated by LACBED.

DISLOCATION MECHANISM OF CHARGE CARRIER TRANSPORT IN SILVER HALIDE MICROSYSTEMS

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In this paper we report on the dominating role of misfit dislocations in the mechanisms of photoinduced charge carrier creation and transport in double structures based on silver halide (AgHal) systems including microparticles and thin layers. We analyzed two types of systems: (i) double structure core-shell particles of around 1 micron in diameter consisting of a crystal AgBr core covered with a thin $AgBr_{(1-x)}I_x$ (x=0.01 - 0.05) layer and (ii) AgBr single crystal / $AgBr_{(1-x)}I_x$ thin film double structure. In both cases under consideration the difference of the crystal lattice parameters gave rise to the creation of misfit dislocations that should influence the main transport properties of the whole system.

We have provided a theoretical analyses of charge carrier creation and transport in mentioned above systems under illumination meaning the presence of misfit dislocations in the top AgHal layer. The charge transfer processes were found to be connected with hopping conduction via dislocation states. It was shown that photoinduced Ag ions transport also comes along the dislocation tube that resulted in the formation of silver clusters at the layer surface.

To prove the proposed theoretical approach we have conducted Maxwell-Wagner effect experimental measurements in double structure particles. The measurements were carried out at the frequency range between 30 Hz and 100 MHz. AgHal particles were insert into a dielectric medium and we analyzed the imaginary part of dielectric loss curve (ε'') versus frequency. The obtained dispersion curve possessed two maxima that gave us possibility to separate the conductivity parameters for both core and the shell structure and to prove the results obtained from the proposed dislocation model. Some experimental details including the role of surface conductivity are also under consideration.

AMORPHOUS SILICON PHASE INFLUENCE ON POLYSILICON ENERGETIC STRUCTURE

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The Effective Medium Approximation (EMA) /1/ is a usually method for estimating the dielectric response for a mixture (in our case polycrystalline silicon compound by crystalline silicon-cSi, amorphous silicon-aSi and voids). From refraction index n and absorption constant spectra (calculated with this method) is possible to evaluate by Tauc /2/ and Cody /3/ models the value for optical bandgap for the material taking into account that it is non-crystalline.

C-Si structure can be modifying by a-Si introducing. So, the optical properties are changed because another phase into c-Si introduce the disorder, or it can said appear an extended defect in c-Si. From $\sqrt{k}$ versus (hω) (Cody/3/)or 1/ hω (Tauc/2/) by a linear fit were evaluated the value for optical bandgap. In both models does make the assumption that the density of state is responsible of spectral dependence of absorption index (which depends on absorption coefficient by the relation $\alpha = 2k\omega / c$).

The voids percent was kept constant zero and it was varied the aSi and cSi percent. The investigated energy is in the range of 1.65 eV to the edge of fundamental absorption. The formula for absorption coefficient demonstrated by Tauc and Cody fit the simulated spectra for k.. The absorption index (represented by f=$\sqrt{k}$) became smaller in the same way as the amorphous silicon percent.

In figure (Cody model) there are represented the calculated values for optical bandgap as a function of a-Si percent. The Tauc model gives greater values for E_g comparatively with Cody model. For the both situation there are a very good fit by the next formula:

$$y = \frac{A_1 - A_2}{1 + e^{(x - x_0)/dx}} + A_2$$

where the parameter values could be seen in the figure. The values of the fit parameters are very closely for both models.

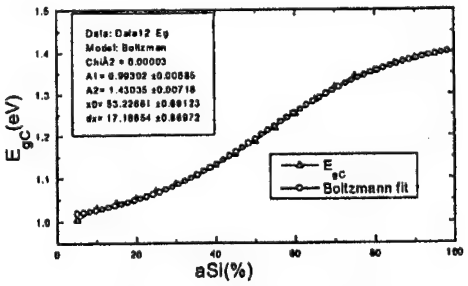

Figure. Fit for E_{gC} (aSi %) function (by Cody)

Cody and Tauc relation in the range of 30 to 90 percent of amorphous silicon can successfully model the polycrystalline silicon. The $\sqrt{k}$ function was linear fitted, and it was evaluated the value for optical gap in the case of variable aSi fraction. The absorption index and energy of optical bandgap increase when amorphous silicon percent increase. The values for $\sqrt{k}$ and the obtained results are in a good agreement with the literature /4/.

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INVESTIGATION OF THE GaAs LAYER EFFECTS ON THE AlGaAs/Si TANDEM SOLAR CELL EFFICIENCY

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The AlGaAs/Si monolithic tandem solar cell is attractive for its high efficiency, low cost and large-area photovoltaic cell from the band-gap-energy point of view. Nevertheless, the main problem of realizing the high efficiency solar cell is the degradation of the minority carrier lifetime of AlGaAs layer. This is caused by the high density of dislocation in the AlGaAs layer on Si due to the lattice mismatch and the difference in the thermal expansion coefficient. Moreover, the minority carrier lifetime is also degraded with the increase of Al composition. In this work a GaAs layer for which electrical properties are investigated is introduced between the top cell and the bottom cell in order to reduce dislocations. The cell performance is optimized, using PC1D simulator, by improving the material and interface quality without altering the cell structure.

OPTIMIZATION OF IMPLANTATION DOSE AND ANNEALING TEMPERATURE IN SILICON WAFERS IMPLANTED As^+ AND ANNEALED BY RTA

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The very-large scale integration (VLSI) technology is characterized by two properties: a high doping activation and smaller dimensions. Those are dependent of several parameters. The implanted ion dose and annealing temperature are the optimized parameters in this paper. For that, several experimental characterization techniques (SIMS, RBS, square resistance and C-V metrie) are used.

Silicon wafers implanted As^+ at different doses (2.10^{14} cm^{-2} - 10^{16} cm^{-2}) and annealed by Rapid Thermal Annealing (RTA) at different temperatures are studied.

A significant redistribution is obtained for high concentration impurities and high temperatures. The optimal recristallisation conditions of implanted layers were: 4.10^{15} cm^{-2} as a dose and 1100°C as annealing temperature.

To have an idea about the diffusion impurities mechanisms in the considered layers, we have proceed with a theoretical simulation (SUPREM) which we have confronted to our experimental results. An important correlation is found between theoretical and experimental profiles for weak and average doses (10^{14} cm^{-2} - 10^{15} cm^{-2}).

THE INFLUENCE OF THE FREE CARRIERS AND POINT DEFECTS ON THE ELASTOOPTIC PROPERTIES OF n - ZnSe CRYSTALS

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ABSTRACT

It is well known that the physical properties of AII - BVI semiconducting compounds depend on many factors, such as the stoichiometry, doping, native defects, free carrier concentration as well as on temperature and pressure (including internal stresses).

Many theoretical and experimental investigations concerning the influence of the free carrier concentration on the physical properties of the n-ZnSe single crystals have been reported recently, but little is known about the influence of the free carriers on their elastooptic properties [1].

In this paper we present the study of the elastooptc constants p_{ij} of n-ZnSe single crystals with different free carrier concentration using Brillouin scattering method. In order to investigate the elastooptic constants p_{ij} of ZnSe crystals, a substitution method proposed by Cummins and Schoen has beeb involved.

Single crystals of n-ZnSe used in this experiment, were grown by high - pressure Bridgman method. After annealing procedure in liquid zinc at different temperatures in the range from 970K to 1370K the ZnSe crystals, shaped to form rectangular prisms, were mechanically polished and chemically etched. Free carrier concentration was estimated using Hall measurements and Raman scattering experiments .

Our Brillouin study yielded a complete set of the elastooptic constants of n - ZnSe crystals with different free carrier concentration and different exciting wavelengths (different incident photon energy). The observed optical dispersion phenomenon of the elastooptic constants of n - ZnSe crystals is consistent with the results obtained by Bairamov et al during the study of the resonant Brillouin scattering in these crystals [2].

It has been also revealed that the increase of the free carrier concentration causes the increase of the absolute value of the elastooptic constants : p_{11} , p_{12} and p_{44} .

Obtained results are discussed in terms of the free carrier concentration (electronic effect), and size effect caused by the existence of the internal stresses, native defects and uncontrolled dopants which may arise in the ZnSe crystals during the growth process [3].

Acknowledgments: This work was supported in part by the research Project of Poznań University of Technology DS 62 - 147.

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EXCESS ELECTRICAL NOISE AT GRAIN BOUNDARIES IN SILICON

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Silicon polycrystalline ignots as well as polycrystalline films are used in different applications, where electrical current noise is significant characteristic of devices and structures. In this research polycrystalline silicon for samples was obtained by casting (ignots) and by Chemical Vacuum Deposition method (films). In the case of Schottky diodes, p-n junctions and resistors made on the bases of polycrystalline silicon with different grain size it was revealed that a natural idea of dependence of the level of the excess current noise on the grain size is justified in the grain size range 0,001 - 1 mm. Also it was established that this dependence correlated with a lifetime versus grain size dependence of the polycrystalline background silicon material. An attempt to establish Hooge-like equation for polycrystalline samples lead to the appearence of lifetime- and concentration dependent coefficient which connected the value of spectral power densi-ty of the excess noise and inverse product of lifetime and square of the current through a sample. Comparision of these data with a well known data available in literature supported the conclusion about grain size dependence of the level of current noise and also showed that the shape of the the spectra of excess noise: 1/f or generation-recombina-tion noise - depends mainly on the tecnological hystory of the samples with the same level of impurity. It's worth to note, that inhomogenity of a certain grain boundary of a small size could not affect the nature of excess current noise generated in the region of grain boundaries in the case of polycrystalline silicon as much as in the case of inho-mogenities of a large surface area like p-n junctions or Schottky diodes.

Hooge-like relation established in this research looks rather prospective in the development of the model of current fluctuation phenomena of extended defects in silicon.

THE EVOLUTION OF METASTABLE DEFECTS ON THE CdS CRYSTAL SURFACE

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Metastable systems of defects and deep levels in semiconductors are intensively studied in order to solve problems of degradation, recombination-accelerated diffusion and some technological questions of modern microelectronics.

Phenomena of metastability were investigated and discussed from the point of view of photochemical reactions [1] and of electron generation effect on the (0001)-face at cooling in the $A^{II}B^{VI}$ compounds while cooling.

The effect of electron generation at cooling of CdS crystals to the temperature of liquid nitrogen was investigated. This effect is revealed in anomaly temperature dependence of the electroconductive surface and is accompanied by the appearance of electron emission into vacuum. The correlation dependencies between conformity of conductive surface changes and of electron emission intensity while cooling were established.

The conductivity decrease takes place at temperature decrease from 450 K to 300 K both as on $(000\bar{1})$ S-face so on (0001) Cd-face. The activation energy is equal to 0.6 ± 0.002 eV and 0.4 ± 0.02 eV for these surfaces, respectively. Usual temperature dependence of equilibrium conductivity takes place for high-ohm CdS-crystals. In the process of further cooling the conductivity of S-face continues to decrease and at T<250 K becomes very small. The conductivity of Cd-face in the temperature range 220-80 K increases more than by 1.5 orders. Electron emission with 3÷5 eV energy from the (0001)-face is observed during this. It decreases by 50% at the fixed 80 K temperature during 90-100 min. The intensity of electron emission sharply decreases to the zero level during the temperature increase to 10-15 K above the temperature of liquid nitrogen. The conductivity decreases by 60÷65%.

The further temperature increase leads to conductivity increase beginning from 130-140 K. The cycles heating-cooling can be repeated on the same sample for many times. The results are completely reproduced at this. The electron concentration in the surface conductive layer at 80 K is equal to $5\cdot10^{17}\div1\cdot10^{19}$ sm^{-3} (at 300 K $n_e < 10^8$ sm^{-3}).

Anomaly temperature dependence and electron emission disappear by IR-light, moreover this decay spectrum coincides with the photocurrent decay spectrum [1]. The coincidence of these decay spectra means that in this temperature range, where the electron emission and anomaly temperature dependence of surface conductivity take place, the holes appear on photosensitive centers.

It is impossible to explain these regularities only by pyroelectric properties of CdS crystals, because the electron emission from S-face is not observed. That's why it is supposed that the evolution of metastable defects is caused both by pyrofield and by the participation of growth dislocation. The availability of Cd-precipitates on the surface of (0001)-face is necessary for the formation of conductive layer with a large quantity of free electrons.

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LOW-TEMPERATURE MECHANO-STIMULATED CHANGE OF CdTe CRYSTALS CONDUCTIVITY.

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Special undoped CdTe singlecrystals were cooled to 77K and were compressed in a single-axis <100> direction (E=1%). The photo- and electroconductivity change of the charge state of the sample's surface and a mechano-stimulated luminescence in the direction perpendicular to the deformation's axis were analyzed.

The correlations of mechano-stimulated conductivity change depending on the direction of the applied external electrical field and the value of the deformation changes were determined. At the initial compression stage (E=0,15%, $V=5\times10^{-8}$ m/s) the conductivity of samples decreases by 18-20%. A value of conductivity doesn't change itself at the fixed value of compression. An uncompression causes a rise of the remained conductivity, the dark value of which is higher than the primary one. The increase of the speed of deformation causes insignificant increase of the remained conductivity value after uncompression.

The change of a polarization of the applied electrical field causes an increase of mechano-stimulated conductivity, the value of which is proportional to the deformation speed. The conductivity value decreases according to an exponential law to the initial value at the fixed value of compression. An uncompression of the sample with a speed of $V=20\times10^{-8}$ m/s causes the change of the charge's state of the surface.

The obtained experimental results are explained from the point of view of dislocation mechanism of defects and charges shifting. In this case the presence of proper point defects and charges, that possess a low symmetry, are taken into account [1]. The similar complexes are formed with a high efficiency during the dislocation movement and they become localized in plains of their slide. The above mentioned complexes are metastable and they keep their properties in the area of low temperatures (~80K). They may be quickly annealed at the room temperature. The correlations between the change of the conductivity and the change of polarization of the applied tension are analyzed considering the crystal unipolarity.

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THERMAL STRAINS AND DYNAMICS OF THEIR RELIEVING BY EXTENDED DEFECTS FORMATION IN EPITAXIAL MULTIVALLEY SEMICONDUCTOR FILMS USING THE GALVANOMAGNETIC EFFECTS ROTATIONAL DEPENDENCE

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Substrate-induced strain in epitaxial thin films has long been recognized as a problem which impacts both fundamental studies and applications. The important feature of multivalley semiconductors with cubically symmetric structure is that the distortion of crystalline structure induced by stresses of different origin leads to a significant semiconductor band structure rebuilding. As it was shown by R. S. Allgaier [1] on the example of n-type PbTe/BaF_2 films, the distortion degree of band structure and, accordingly, the value of elastic strains can be estimated in such a case by using the four-coefficient weak-field magnetoresistance (WFMR) measurement technique.

Strain value and strain relaxation dynamics after many temperature cycles between room temperature and 77K have been investigated for n- and p- PbTe and PbSnTe epitaxial layers with different thicknesses on BaF_2 substrates. Obtained results correlate well with carrier concentration and mobility changes induced by extended defects appearing due to plastic deformation which occured in each cycle. There are three trends in the data that occur as the number of thermal cycles is increased: (1) the transfer factor F which indicates the ratio of the density of carriers in the [111] valley to each of the other valleys is greater than 1 in the as-grown sample and approaches unity (while thermocycling); (2) the carrier concentrations measured at both 77K and room temperature increase almost linearly; and (3) the mobility drops rapidly during the first few temperature cycles and then decreases at a slower rate. The observed effects are ascribed to the extended defect density enhancement with increase in the number of thermal cycles. After the first few thermal cycles no new thermal-strain-relieving dislocations are created.

This technique seems to be a convenient and reliable mean to study dynamics of extended defects creation for thermal-strain-relieving in heteroepitaxial layers of multivalley semiconductors.

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THE PECULIARITIES OF THE INITIAL STAGE OF SINGLE AXIS LOADING IN SEMICONDUCTORS AND DIEIECTRICS

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In_4Se_3 semiconductor monocrystals with 4×4×8 mm size were subjected to a single axis pressure with a constant velocity $\varepsilon \sim 10^{-4}$ s^{-1} at the room temperature in a vacuum chamber on the device for mechanical investigations .According to the received loading-deformation diagrams that at small deformations beginning from ε~0,05% the deviation from the linear loading at a constant velocity of deformation was observed .Velocity and temperature of the investigation don't noticeably influence the G-E diagram course. Only annealing at certain temperatures leads to increase of linear loading(within elasticity).

LiF, NaCl dielectrics. Plastic deformation of ion crystals occurs because of motion and multiplication of dislocations. Dislocations in ion crystals are charged. The value and sign of the charge on the surface of the deformed sample depend on the type of the doped admixture, velocity of the deformation, ionized irradiation and temperature at which the experiment is carried out. Synchronous measuring loading-deformation of diagrams and kinetics of a surface charge accumulation showed that a certain correlation exists between them. The charge of one sign appears before the beginning of flowability and then the inversion of charge sign takes place. On the second plot the charge is determined by the type of the admixture.

The investigations carried out on the LiF monocrystals showed that the dislocations appear before the beginning of flowability on the surface of the deformed sample. Their quantity increases at increasing of the deformation degree (ε - 0,03-0,05%). At lauer by lauer etching it was revealed that the dislocation density lineally decreases to the value which was on the surface of non-deformed sample at the ~100mkm distance from the sample surface. The peculiarities of the initial stage of deformation of semiconductors and dielectrics that were investigated above can be explained by the reduction of energies of formation and moving of point linear defects near the free surface as well as by the influence of mirror image forces.

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10:40 **coffee break**	10:20 **coffee break**	10:20 **coffee break**	10:50 **coffee break**	10:20 **coffee break**
11:10 VDOVIN 11:50 PICHAUD 12:30 *KĄTCKI*	10:50 PIZZINI 11:30 SEIBT 12:10 *ALIPPI*	10:50 YAMASHITA 11:30 BULATOV 12:10 *YONENAGA*	11:20 ROUVIERE 12:00 SALVIATI	10:50 *LEIPNER* 11:10 *STEINMAN* 11:30 Closing
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